
G.M. van Hoesve-Brouwer

TEACHING STRUCTURES
IN CHEMISTRY

*An Educational Structure for
Chemical Bonding*



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An Educational Structure for Chemical Bonding

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TEACHING STRUCTURES IN CHEMISTRY

An educational structure for chemical bonding

CHEMISCHE STRUCTUREN IN ONDERWIJS
Een didactische structuur van chemische binding
(met een samenvatting in het Nederlands)

Proefschrift

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Contents

INTRODUCTION	1
1 A MATTER FOR INVESTIGATION	5
1.1 A Chapter on Chemical Bonding	6
1.2 Sources of Confusion	11
1.3 Analysis of the Sources of Confusion	14
1.4 Recommendations for Revision	17
1.5 Results and Questions for Investigation	20
2 REFLECTIONS ON CHEMICAL BONDING	25
2.1 Source of Confusion: Chemistry Context or Physics Context	25
2.2 The Role of Quantum Mechanics	30
2.3 Reductionism or Pluralism	33
2.3.1 Reductionism, strong or weak	33
2.3.2 Structure and shape: one theory or plurality of theories	35
2.4 Pluralism: Contexts Alone and Together	38
2.4.1 Periodic Table and combination of contexts	38
2.4.2 Formation of methane, change of context or hybridization	40
3 CHEMICAL BONDING AND WORKING WITH MODELS	45
3.1 Models and the Corpuscular Nature of Matter	45
3.1.1 Models, formal and canonical	45
3.1.2 Representing reality	47
3.2 Corpuscular Models in Three Textbooks	50
3.3 Characteristics and Introductions of Models Combined	54
3.3.1 Characteristics of models in practice	54
3.3.2 Introducing the use of models in chemistry education	55
3.3.3 Model characteristics and methods of introducing a model	57
3.4 Chemical Bonding and the Use of Models	58
3.5 Molecular Shape and the Use of Models	63
3.6 Discussing Models and Contexts	65
3.6.1 Views on model characteristics	66
3.6.2 Views on corpuscular models in chemistry education	67
4 EDUCATIONAL ANALYSIS AND EDUCATIONAL EXPERIMENT	71
4.1 Developing Educational Texts and Contexts	71
4.2 The Chemistry Context of the Molecular Structure Theory	75
4.3 Molecular Models and Structural Formulae	79
4.3.1 Shifting the limits of perception	79

4.3.2 Correspondence terms; structural formulae as molecular models	81
4.3.3 Structural formulae: representation of properties and molecular models	82
4.3.4 Teaching the relativeness of structural formulae	84
4.4 Building Contexts	85
4.4.1 Procedures in scientific practice	86
4.4.2 Acquiring knowledge and the syntax of fluid enquiry	88
4.4.3 Procedures of scientific writing	89
4.4.4 Historiography and educational narrative	90
5 GETTING ACQUAINTED: AN EDUCATIONAL EXPERIMENT	93
5.1 The Educational Text	93
5.1.1 Objectives	94
5.1.2 Content	95
5.1.3 Narrative	97
5.2 The Substances and Their Reactions	98
5.2.1 Properties of the substances	98
5.2.2 Substances and structural formulae	100
5.2.3 Structural formulae and reactions	102
5.3 A Narrative with Episodes	103
5.3.1 The Pelouze episode	103
5.3.2 The Van 't Hoff episode	104
5.3.3 The Lewis episode	106
5.3.4 The Yardley episode	107
5.3.5 The fifth episode and the global context	108
5.4 The Assignments in the Educational Text	109
5.4.1 The purpose of the assignments	109
5.4.2 Observation report on the assignments	112
5.5 The Titration Assignment	113
5.5.1 Mobilizing prior knowledge	114
5.5.2 Calculation sequences	116
5.5.3 Consequences of using a pH meter	117
5.6 Titration, Correspondence Terms and Sequence of Contexts	119
5.6.1 Titration in different contexts	120
5.6.2 Contexts in the episodes and contexts in an educational structure	121
6 CREATING KNOWLEDGE IN AN EDUCATIONAL EXPERIMENT	125
6.1 Adjustments for a Second Experiment	125
6.1.1 Global context, communication and closing episode	125
6.1.2 Regulating the openness	127

CONTENTS

6.1.3 Structural formulae, dashes and sequence of contexts	130
6.2 The Trial with Recontextualization	132
6.2.1 A question to guide the search	132
6.2.2 A question to guide the selection	134
6.2.3 A question to guide the writing	136
6.3 The Trial with the Hydrogen Bond	138
6.3.1 Hydrogen bonds depicted	138
6.3.2 Hydrogen bonds oriented in space	141
6.4 Reflections on Teaching Structures	148
6.4.1 Teaching structure for creating knowledge	148
6.4.2 Considerations on an educational structure	150
6.4.3 An introduction to the molecular structure theory	151
6.4.4 A teaching structure on the basis of reactions	152
6.4.5 Introduction of a new educational text	154
EPILOGUE	157
REFERENCES	161
APPENDIX: The Story of a Substance	167
SAMENVATTING	187
DANKWOORD	193
CURRICULUM VITAE	195

Introduction

Chemistry has its own specific way of looking at the world. It entails observing matter and its processes and describing these observations in terms of substances and their reactions in both practical and theoretical notions. The chemical way of looking at things takes a long time to acquire. In their professional life, chemists are proficient in this chemical way of looking at the world. Wherever they are working, they use knowledge and procedures they have learned at university or institutes of higher or vocational education. Before that, in most countries, they will have acquired a grounding in chemistry at secondary school.

Learning chemistry at school implies that chemical knowledge and procedures are taught as considered appropriate for students at that level of education. One of the topics of the advanced level, i.e. chemical bonding with its theories and models is usually introduced at the end of the upper secondary school curriculum. The traditional content of the chapter or chapters on chemical bonding is based on the objective of achieving a certain level of knowledge supposed to be required by the university curriculum. As only a few students will continue studying chemistry, one might question whether the chemical content of the topic is relevant for all students. However, experience in working with theories and models acquired when learning chemical bonding can be regarded as useful for students before entering university studies. In practice, students as well as teachers come up against difficulties when learning and teaching the essential concepts. These difficulties could be caused by a specific conceptual structure or by the traditional content. In educational research, both can be brought up for discussion. In this thesis, I report the results of such an educational research project which pertains chemical bonding at pre-university level.

My experience as a chemist and as a teacher is the background against which I entered into educational research. I studied biochemistry in a period when this science was being established as a separate branch of chemistry. In biochemistry, structure is a dominant concept, as substances and their biochemical activities are preferably described in terms of structure-property relations, and in the form of lock-and-key representations. While devising educational texts for the research project, I have been influenced by my education in biochemistry and organic chemistry.

Before I started teaching at school I coached students for several years. In my experience coaching a student is a good way to learn how to teach a certain topic. One has better opportunities for personal interchange and direct response. Also more time is available to reflect and reformulate together.

During most of the period I was active as a teacher, I was also a member of a team of editors of a chemistry textbook series, CHEMIE. I joined the team because of my interest in communication in written and pictorial form.

The team of editors is called 'Gebruikersredactie' and consists of teachers who use the textbooks themselves ('gebruiken' - to use). The first task of the Gebruikersredactie was

to edit the texts written by the 'Commissie Moderniserend Leerplan Scheikunde' (CMLS, the Netherlands Committee for Reform of the Chemistry Curriculum). The first edition of the textbook series can be seen as a continuation of the developmental work of the CMLS. When the second edition was to be published, the 'Gebruikersredactie' was asked to revise and, if necessary, rewrite the texts using their own experiences and those of fellow teachers. I was specially involved in the chapters on organic chemistry and biochemistry. Before the work on the third edition started I left the 'Gebruikersredactie', but I remained involved in the work by participating in a small scale project. This project started when the Department of Chemical Education of Utrecht University and Wolters-Noordhoff, the publisher of the series, agreed to cooperate. The objective of the small scale project was to analyze a chapter that was to be revised for the third edition, i.e. 'Hoofdstuk 10', the chapter on atomic structure and chemical bonding. This chapter is part of the textbook for the 13th year. My motive for participating in the small scale project was to learn more about the chemical concepts and procedures incorporated in textbooks. By looking into that particular chapter, I also wanted find out an answer to the question I had experienced as a teacher why chemical bonding is considered to be a difficult topic in school chemistry.

So both as a learner and teacher of chemistry, I became involved in educational research into chemistry and chemistry education.

The Department of Chemical Education considered that the small scale project and the subsequent PhD research project on chemical bonding fitted in with the programme of concept developmental research of the Centre of Science and Mathematics Education in which the Department is participating. The general characteristics common to the research projects of the Department include a qualitative research approach, a critical analysis of the chemical content in question, an educational experiment in the classroom with texts designed for that experiment, analysis of classroom discussions between students and teachers when working with the texts and, finally, a detailed evaluation of the results. Research on chemical education at secondary level is carried out on: conceptual structures in traditional school chemistry, an introduction into chemistry based on preparation of products in a societal context, and teaching of electrochemical concepts and procedures. Earlier educational research was on stoichiometry, mole concept, chemical equilibrium and molecules and atoms in elementary chemical education. The Chemical Bonding research project is in line with these studies because they concern the particulate nature of matter and the corpuscular hypothesis regarding molecules and atoms. I left teaching and joined the Department on Chemical Education in 1990 to participate in the Chemical Bonding research project. The research reported in this thesis comprises both the small scale project when I was still working as a teacher, and the project on chemical bonding carried out in the period 1990-1995. The following is an overview of the chapters of the thesis.

The first chapter reports the analysis of 'Hoofdstuk 10' and other findings of the small scale project. The analysis focuses on the framework and function of concepts with regard to atomic structure and chemical bonding. The results of the analysis show that the conceptual structure underlying the approach to teaching chemical bonding is characterized by at least one major inconsistency which we have called the *gap*. This is described as the gap between the model of a free atom and that of a bonded atom, and as the gap which arises when chemical bonding is approached from a point of view of physics .

The research project on chemical bonding is a continuation of the small scale project. Therefore, the analysis of Hoofdstuk 10 is to be regarded as the starting point of the educational analysis to be pursued in the research project. At the end of the first chapter the aims of the research project and the questions to be answered in the following chapters of the thesis are formulated.

Chapter 2 gives a further educational analysis of the text on chemical bonding and goes more deeply into a reason for inconsistencies in the sequence of concepts as in Hoofdstuk 10. This sequential presentation of free and bonded atoms is found in other secondary school textbooks and in a university textbook as well. This sequence is linked to a 'theory first' approach and the idea that physics is the fundamental science, which underlies the reductionistic approach. I present arguments indicating that not all chemists are convinced of the applicability of the reductionistic approach and, that chemical structure cannot be derived from first principles on a strictly theoretical basis. The Periodic Table is discussed as an example of a successful combination of phenomena and theories from chemistry and physics contexts. The formation of a methane molecule is discussed as an example of a combination of phenomena and theories within the chemistry context.

Chapter 3 continues the educational analysis and focuses on working with models of molecules and atoms. Working with models in education is linked to a two-step thesis of reduction. To begin, the hypothesis of the particulate, or as I prefer to call it, the corpuscular nature of matter must be accepted. Only then can models of the corpuscles, i.e. molecules and atoms, be introduced and used. A teaching problem which I refer to as the *minima naturalia* dilemma is linked to the first step of accepting corpuscularity. Three methods of introducing the use of models are discussed: a single-model approach of presenting just one model, an approach of introducing successive models in historical order or progressing from simple to complex, and a multi-model approach using models side by side to convey the idea of the relativity of models. I also analyze how models and the use of models are introduced in three different textbooks.

Chapter 4 links the educational analysis of the foregoing chapters to the educational experiments in the cyclic procedure of educational research and the development of educational texts.

As a result of the educational analysis reported in Chapters 2 and 3, the focus is on the chemistry content of the educational text with regard to replacing the physical introduction by a chemical introduction, i.e. the molecular structure theory. The structural formulae can be introduced as a suitable means of conveying the relativeness of models. Guidelines are needed for writing the educational text. These guidelines are found in the context of chemistry as a science, in the rules for writing scientific texts and in the principles of writing a historical narrative.

The account of the educational text is given in Chapter 5. First the objectives of the text are discussed in relation to the guidelines. Then I give my arguments for choosing the substances maleic acid and fumaric acid, and my choice of people and their publications for episodes of the narrative in the framework of creating knowledge. In the educational experiment, the assignments in the educational text are used as a tool to gather research material from discussions among students and their teachers as they work with the text. The results of the first round of trialling in the educational experiment are presented and discussed. Special attention is given to the results of the titration assignment. A tentative educational structure on chemical bonding is proposed.

Chapter 6 discusses the revision of the educational text for a second round of trialling. One result is the adjustment of the design of the closing episode according to the guidelines for designing educational texts. The assignment on the hydrogen bond is discussed in detail for the interpretation of the research material in the second round of the educational experiment. The chapter ends with reflections on the tentative educational structure of chemical bonding which resulted from the educational analysis and experiment. Two suggestions for the application of the educational structure are given, one is using a different sequence of concepts when introducing the molecular structure theory in a lower level of secondary education, and the other is introducing chemical bonding by starting from reactions instead of substances. To conclude some remarks are made on the implementation of an educational text developed as part of an educational research project.

1 A Matter for Investigation

In this chapter I report on a small scale project entitled "Revision of Hoofdstuk 10". The participants in this project were W. de Vos, E. Vroemen and the author of this thesis. All three have experience as teachers and as writers of educational texts. The first also lent support to the project with experience in chemistry education research.

The aim of the project was to contribute to the preparation of the third edition of the textbook 'CHEMIE 5/6V'¹, focusing specifically on a topic called Atomic Structure and Chemical Bonding. CHEMIE 5/6V is part of the series of chemistry textbooks that is most widely used in the advanced level of secondary schools in the Netherlands. In the second edition, the topic on chemical bonding is dealt with in "Hoofdstuk 10: Atomen alleen en te zamen" ("Chapter 10: Atoms alone and together"). I will use the expression 'Hoofdstuk 10' to refer to this chapter and to distinguish it from the chapters in this thesis.

The topic was selected for analysis in the project because it was regarded as difficult by teachers (users of the book) and by the Gebruikersredactie (a team of authors/teachers who also use the book themselves). Furthermore, the topic fitted in with the research programme of the Department of Chemical Education of Utrecht University. This programme focused, among other things, on the development of chemical concepts, for instance, chemical equilibrium (Van Driel, 1990). Some problems related to the particulate nature of matter had already been addressed in the thesis of De Vos (1985).

The limited time allotted to the project restricted the scope and the depth of the analysis. Therefore, it was decided to concentrate on those sections of Hoofdstuk 10 which specifically deal with atomic structure and the formation of molecules.

By way of introduction, Section 1.1 will give an overview of parts of Hoofdstuk 10 selected with regard to the structure of free atoms and the formation of molecules, i.e., the atoms "alone" and "together". In Section 1.2 I report on inconsistencies found in Hoofdstuk 10. I call these inconsistencies *sources of confusion*. I analyze the sources of confusion in Section 1.3. The suggestions we made to the Gebruikersredactie for improving coherence or for overcoming inconsistencies are discussed in Section 1.4. In Section 1.5 I present two results of the project, viz., a proposal for a revised chapter on atomic structure and chemical bonding, and a proposal for the PhD research project "An Educational Structure of Chemical Bonding".

¹ CHEMIE 5/6V: Smilde, J., G.M. Van Hoeve-Brouwer, L.O.F. Pieren, K. Klosse, H. Van Dieten and H. Wessels (1985a and b). *Chemie 5/6vwo 1-8* and *Chemie 5/6vwo 9-11* (2nd edition) Groningen, Wolters-Noordhoff.

1.1 A Chapter on Chemical Bonding

The chapter on chemical bonding, Hoofdstuk 10, is part of the second edition of a chemistry textbook, CHEMIE 5/6V (1985), intended for the highest form of upper secondary school (pre-university education). It is the closing chapter on the theoretical aspects of chemistry.

First, I briefly mention the concepts which have been introduced in earlier units of CHEMIE (second editions)²:

- Rutherford's model of the atom, i.e. a relatively very small and heavy nucleus consisting of positively charged protons and neutral neutrons, surrounded by an electron cloud consisting of negatively charged electrons (CHEMIE 3V/H, 1983, p.146);
- a conception of the chemical bond as a result of mutual attraction between the positive nuclei and the negative electrons of participating atoms (CHEMIE 3V/H, 1983, p.139);
- an atomic (covalent) bond consisting of a shared electron pair that holds the two positive remaining parts of the atoms together. The electron pair is depicted by a dash (CHEMIE 4V, 1984, p.11, 12);
- the ionic bond constituted by the attraction between positive and negative ions (CHEMIE 4V, p.44);
- the metallic bond described as positive remaining parts of the atoms held together by negative free electrons (CHEMIE 4V, 1984, p.178);
- the bond between molecules resulting from vanderwaals forces (CHEMIE, 4V, 1984, p.10);
- the intermolecular hydrogen bond occurring between molecules containing hydrogen atoms bonded to an oxygen or a nitrogen atom (CHEMIE 4V, 1984, p.96).

In Hoofdstuk 10 it is assumed that students have learnt and understood these concepts which have been taught two or three years earlier. At the same time, however, it is reasonable to assume that a certain amount has been forgotten. Hoofdstuk 10, therefore, offers both a recapitulation and an expansion of knowledge already taught.

Hoofdstuk 10 consists of eight sections. The first four sections discuss the periodic table and atomic structure, three cover bonding in elements and compounds, and the last section deals with reaction mechanisms. No experiments are included, although the empirical basis of data is referred to. For instance, the experiment of Franck and Hertz is mentioned when ionisation energies are introduced. It is assumed that some chemical properties of the elements are known. Results of experiments are available in the form

² The series CHEMIE (2nd edition) for advanced level chemistry education consists of: CHEMIE 3V/H (Pieren, Van Dieten, Van Hoeve-Brouwer, Klosse, Smilde, Wessels and Hondebrink, 1983); CHEMIE 4V (Van Dieten, Pieren, Van Hoeve-Brouwer, Klosse, Smilde and Wessels, 1984); CHEMIE 5/6V (Smilde, Van Hoeve-Brouwer, Pieren, Klosse, Van Dieten, and Wessels, 1985a, b).

of data compiled in a schoolbook version of the Handbook of Chemistry and Physics, referred to as "BINAS tabellenboek" (1977, first edition; 1986, second edition).

The sections on atomic structure and the section on the formation of molecules can be summarized as follows:

Section 10.1; The periodic table and atomic structure. The introductory section discusses the periodic table and briefly recapitulates atomic structure. The framework of this section is illustrated by the introductory sentences:

"In every science attempts are made to introduce order into the abundance of data. Theories are formulated to describe phenomena and, if possible, to make predictions." (CHEMIE 5/6V, 1985, p.268)³

The periodic table is presented as an example of such order. The arrangement of the elements in the periodic table is said to be based on increasing atomic mass and on periodically occurring similarities in chemical properties. The structure of the atom corresponds to Rutherford's descriptions: a small positively charged nucleus surrounded by a negatively charged electron cloud. Atomic structure concepts in relation to the periodic table are repeated and extended. The atomic number of an element is equal to the number of protons in the nucleus and to the nuclear charge, Z . Atomic mass is defined as the sum of the nuclear particles, i.e., protons and neutrons.

Section 10.2; The electron cloud. The section starts by stating that (i) a neutral atom has the same number of electrons as its number of protons in the nucleus, and (ii) an electron and a proton have the same but opposite charge. Attention is drawn to the electron cloud, because:

"On the basis of many observations, we assume that the electron cloud determines the chemical properties of the element. Therefore, it is worth while to examine its structure." (CHEMIE 5/6V, 1985, p.270)⁴

The ionisation energy is introduced as the energy required to remove an electron from an atom. Reference is made to a table in BINAS (1977) with ionisation energies of about thirty elements. Students are asked to draw a diagram of the ionisation energies (eV) of the first electron of the atoms of H up to and including Ca, and to plot it against the atomic number. Another diagram, presented in a figure, is the result of plotting the logarithmic values of the subsequent ionisation energies of sodium against the number of electrons removed. This figure shows that the electrons of the sodium atom fall into three groups according to their ionisation energies: the electron *leaving first* in the *lowest* group. The next figure shows that the electrons are located on energy levels and that a *small* ionisation energy of an electron corresponds to a *high* energy level.

³ "In elke wetenschap wordt ordening aangebracht in de stroom van gegevens. Men stelt dan theorieën op om de verschijnselen te beschrijven en eventueel voorspellingen te doen." (CHEMIE 5/6V, 1985, p.268)

⁴ "Op de grond van veel waarnemingen nemen we aan dat de elektronenwolk de chemische eigenschappen van het element bepaalt. Een onderzoek naar de bouw ervan is dan ook zinvol." (CHEMIE 5/6V, 1985, p.270)

Electrons in other elements ranging from H to Ar have been grouped in a similar manner. The number of electrons which can be located on a certain energy level is said to be derived from the ionisation energy data. However, in order to understand why, in the case of potassium, the fourth energy level is already used although the third level has not yet been filled up, the "energy model must be refined" (CHEMIE 5/6V, 1985, p.272)⁵.

Section 10.3; Atomic structure: the size of the atom. The relation between the ionisation energies and the dimensions of an atom is introduced by means of Coulomb's Law, assumed to be known from physics lessons. The energy required to remove an electron from a neutral atom is said to be determined by the charge of the nucleus, by the number of (remaining) electrons, and by the distance of the electron in question from the nucleus (CHEMIE, 5/6V, 1985, p.273). A figure shows the *energy of the first electron* of about sixty atomic species plotted against their atomic number (see Figure 1.1). Again, it is stated that a high energy level of an electron corresponds to easy removal of an electron, whereas a low energy level means that much energy is required to detach that particular electron.

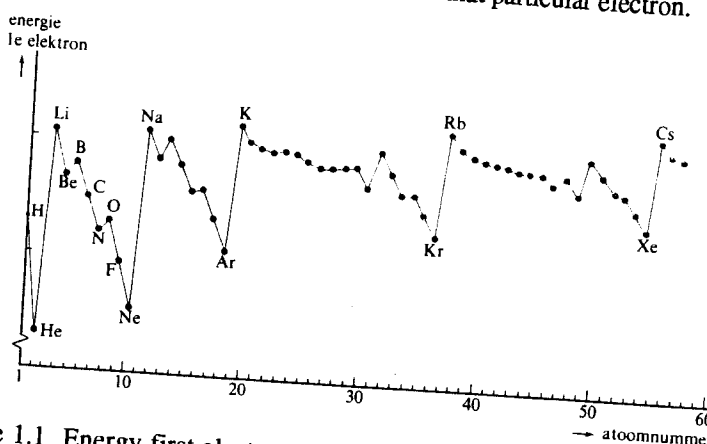


Figure 1.1 Energy first electron against atomic number (CHEMIE 5/6V, 1985, p.273)

According to Coulomb's law, it is assumed that an electron with a small energy value must be situated at a large distance from the nucleus. This leads to the assumption that the energy levels introduced in Section 10.2 correspond to domains at different distances from the nucleus. The representation based on distances from the nucleus is called Bohr's model of the atom. It is mentioned that Bohr derived the existence of energy levels from spectra. It is concluded from these spectra that an electron can absorb only certain amounts of energy and that energy can only be supplied or given up in certain small fixed amounts called quanta. Reference is made to quantum mechanics as a modern theory of the atom. Calculations with the energy quanta and some results

⁵ "(...) moet ons energiemodel worden verfijnd." (CHEMIE, 5/6V, 1985, p.272)

of such calculations are discussed, e.g. a relation between energy transitions and the wave length of the emitted light.

The number of energy levels in an atom is the main determinant of the dimensions of the atom: the greater the number, the larger the atom. Filling up one energy level, however, causes the atom to become smaller because of the increasing nuclear charge. It is pointed out that distances between atoms in crystals have been measured and that, as a result, the radii of certain atoms and ions have been determined. The dimension of the electron cloud of an atom is given by its vanderwaals radius.

Section 10.4; Atomic structure: the valence electrons. The irregular pattern of Figure 1.1 suggests that the second energy level consists of several levels close to each other. Referring to spectra, a refinement of the model of an atom is given by introducing spin as a property of an electron. The spin is associated with a whirling top, i.e. electrons are supposed to rotate around their axis. This is represented with arrows in what is called an energy diagram. Two electrons with the same energy and having opposite spin are called an electron pair. A model for the structure of the electron cloud is now constructed for each atom by filling the energy levels from the lowest level up.

" The electron furthest from the nucleus, is located at the highest energy level; it is the first to be removed when ionisation takes place." (CHEMIE 5/6V, 1985, p.276)⁶

Filling up of the energy levels starts with the hydrogen atom and continues with successive atoms in accordance with the following rules:

- the subdivision in and the naming of *s*, *p*, *d* and *f* energy levels;
- the occurrence of electrons in pairs, except in some cases when sublevels of the same energy are to be filled.

Furthermore, there are two notation systems, viz. with arrows in diagrams and with symbols, such as $1s^2 2s^2 2p^6 3s^1$, both representing what is called the electron configuration of an atom.

When the filling up procedure has reached potassium in the fourth period, the electron configurations are related to the position of the atoms in the periodic table. It is stressed that atoms in the same group of the periodic table have the same electron configuration in the highest energy level. The electron configurations of the elements following potassium are discussed in relation to their position in the periodic table.

Only electrons in the highest energy level, called valence electrons, are considered to be relevant for the chemical properties. Attention is paid to elements which easily form positive ions and have only *s* electrons in the highest energy level. Other elements are pointed out which can easily form negatively charged ions by filling up a *p* level. It is said that atoms can also fill up an incomplete *p* level by forming molecules. A comment states that the energy levels as described are those of free atoms and that the position of energy levels of atoms or ions in compounds may be slightly different, especially for sublevels close to each other. The example

⁶ "Het elektron dat zich het verst van de kern bevindt, zit in het hoogste energieniveau; het wordt bij ionisatie het eerst verwijderd." (CHEMIE 5/6V, 1985, p.276)

is given of the elements scandium to zinc most of which are bivalent: in compounds the $4s$ level seems to be higher than the $3d$ level, whereas, according to the filling-up procedure of the atoms, scandium's last electron has been placed in the $3d$ level which is higher than $4s$ level. The section ends with an optional passage on the historical development of quantum theories.

Section 10.5; Molecules. The opening paragraphs of the section say:

"A hydrogen molecule consists of two H atoms, that is, 2 nuclei and 2 electrons.

An H atom has 1 electron in the $1s$ -level. This applies also for the other H atom with which a molecule H_2 has to be formed. Both electrons form an electron pair which lies as a shared electron cloud between both positive nuclei. This shared electron pair has a lower energy value than both single electrons together." (CHEMIE 5/6V, 1985, p.284)⁷

The formation of a hydrogen molecule is represented in an energy diagram with the single arrow notation for the electrons of the free H atoms and the opposite spin notation for the electron pair of the hydrogen molecule. The electron pair holding both nuclei together is called a bonding electron pair. This is represented in the structural formula with a dash between the symbols: H-H.

In a discussion of the hydrogen chloride molecule the following aspects are mentioned:

- the shared bonding electron pair is formed by the one electron of the hydrogen atom and the unpaired electron of the $3p$ level of the chlorine atom;
- there are four electron pairs around the chlorine atom, i.e. one bonding and three non-bonding pairs;
- the chlorine atom obeys the rule of eight, or octet rule, according to which atoms in covalent compounds have eight electrons in the highest energy level.
- the electron formula is introduced: the symbol of the element is surrounded by four dashes representing the bonding and non-bonding electron pairs.

Electron formulae can be drawn by counting and rearranging valence electrons.

Furthermore, it is implied that the four valence electrons of the carbon atom are equivalent in the formation of methane. The energy of the $2s$ and $2p$ sublevels in the carbon atoms is averaged leading to four equivalent C-H bonds. Valence electrons form shared electron pairs with the electrons of the H atoms. These are indicated with bonding dashes in structural formulae. Double and triple bonds are represented by two or three dashes respectively.

It is stressed that not all compounds can be described according to this theory. For instance, some complex compounds, such as the copper tetraamine ion in which the central particle is surrounded by ions or molecules, do not follow the rule. Another example is PCl_5 . In the structural formulae of these examples the bonds are nevertheless represented with a dash.

⁷ "Een molekuul waterstof bestaat uit twee H atomen, dus uit 2 kernen en 2 elektronen. Een H atoom heeft 1 elektron in het $1s$ -niveau. Dit geldt ook voor het andere H atoom, waarmee een molekuul H_2 moet worden gevormd. De beide elektronen vormen nu een elektronenpaar dat als een gemeenschappelijke elektronenwolk tussen de beide positieve kernen ligt. Dit gemeenschappelijke elektronenpaar heeft een lagere energie dan de afzonderlijke elektronen samen." (CHEMIE 5/6V, 1985, p.284)

The remaining sections of Hoofdstuk 10 deal with:

- the polar bond with the concepts of electronegativity and dipole moment and with the partially ionic character of the polar bond (Section 10.6);
- mesomerism with the various electron distributions which can be drawn up for the mesomeric structures, e.g. in the carbonate ion (Section 10.7);
- reaction mechanisms, with the assumption that reactions take place in steps. This is represented with equations of the various reaction steps using structural formulae as well as electron formulae. Examples are the formation of esters and the reaction of CH_3Cl with OH^- (Section 10.8).

The bond in a hydrogen molecule introduced in Hoofdstuk 10 is called a covalent bond. The bond types in the remaining sections may be regarded as variations of such covalent bonds.

In Hoofdstuk 10, a chapter on chemical bonding, the expression "chemische binding" (chemical bonding) is not used in the text. There is a weak link to substances and reactions. The formation of a molecule is presented as a consequence of the atomic structure; it is not linked to chemical phenomena.

1.2 Sources of Confusion

In the previous section I described those concepts of Hoofdstuk 10 which are considered relevant for the discussion of the text of Hoofdstuk 10 in this and the following sections.

With the objective of a revision of the topic in mind, we went through the text to find out whether the presentation of the concepts was coherent. From the point of view of critical teachers we looked for inconsistencies which might confuse the students. I call some of the inconsistencies we found *sources of confusion* (SC). This section discusses nine such sources. I will describe each source of confusion as it emerged from looking into Hoofdstuk 10 during the project.

It will become clear that the main source of confusion concerns the discrepancy between the section on the formation of molecules and the previous sections on the structure of the atoms.

SC 1. We found an inconsistency between the diagram with the logarithm of the ionisation energies of the eleven electrons in a sodium atom and the diagram with the energy levels of the sodium atom. The diagram with the logarithm of the ionisation energies is required to divide the electrons into groups. A figure of this diagram shows, in the *lowest* band, a *small* value for the ionisation energy for the first electron, subsequently, a broad band with the values of the next eight electrons and, on top, the *highest* band with a *large* value for the last two electrons to be ionized. The order is 1-8-2 from bottom to top. However, in the following text a description and a figure is given

of another diagram, *viz.* with energy levels. The reasoning, going from bottom to top, is as follows: the electrons with the *large* value for ionisation energy are on a *low* energy level; the electron with the *small* value is on a *high* energy level. The order is now 2-8-1. Source of confusion no. 1 is this tangled combination of high-low and small-large in both diagrams.

SC 2. The second inconsistency was spotted when considering two other diagrams. The plot of the *ionisation energies* of the first electrons of the atoms H to Ca against the atomic number is to be compared with the plot of the *energy* of the first electron of the first sixty elements against their atomic numbers (cf. Figure 1.1). The two plots turn out to be each other's mirror image, *i.e.* *high* in one figure corresponds to *low* in the other: this is source of confusion no. 2.

SC 3. The next source of confusion regards the switch from energy level to distance. Ionisation energy data are used to construct an energy model of the atom and to attribute electrons to energy levels. The electrons of some of the first twenty atoms are depicted as dots on lines representing the levels. However, after the introduction of Coulomb's law, the ionisation energy of an electron is interpreted in terms of the distance of that electron to the nucleus. Figure 1.1 is incorporated to make it appear plausible that withdrawing an electron from an atom more easily has to do with a greater distance of that electron from the nucleus of the atom. Source of confusion no. 3 is that energy level diagrams refer to a zero point at infinite distance from the nucleus, whereas the nucleus *is* the zero point in the representation using distances from the nucleus.

SC 4. Bohr's model of the atom offers also a source of confusion, SC 4. In a figure the energy levels of the hydrogen atom are visualized as segments of concentric circles. It is not made clear that this figure is applicable only in the case of hydrogen. The suggestion is made that other atoms may be represented with the same diagram by distributing more electrons over the circles. The image of an atom with circular, and eventually spatial, dimensions is stressed by the attention paid to the various possibilities of radii (atomic, ionic, vanderwaals) in the text and in an accompanying figure.

SC 5. Source of confusion no. 5 is related to the spin. A model of the structure of the electron cloud is to be constructed with energy levels corresponding to specific distances from the nucleus. The filling-up procedure requires the concept of spin as a property of electrons for (i) a description of the model and (ii) a notation with arrows. However, this property seems to imply that Coulomb's law is declared invalid for two electrons with opposite spin as they can form an electron pair.

SC 6. The next source of confusion is the *4s-3d* dilemma. A description in terms of distance to the nucleus is the following. According to the filling-up procedure the

electron in the highest energy level is the furthest from the nucleus and this electron will be the first to be removed in ionisation. The electron in the $3d$ energy level for the scandium atom must be at a greater distance to the nucleus than the two electrons in the $4s$ energy level, following the rule that a $3d$ level is higher than a $4s$ level. However, according to ionisation energy measurements, the two electrons in the $4s$ level are removed first. From this it can be concluded that these are the electrons at the greatest distance from the nucleus.

SC 7. Source of confusion no. 7 arises when valence electrons are introduced. The electrons in the highest energy level are called valence electrons and they are considered to be relevant to the chemical properties. However, it is not made clear which levels or sublevels are involved and what number of valence electrons is possible; it might be two (a pair), six (6 electrons in a p level), eight (octet rule) or ten (10 electrons in a d level). Moreover, the implication is that the electrons in the highest energy level will be located on the outside of the atom.

SC 8. The valence electrons are mentioned with regard to the tetravalency of the carbon atom in a carbon compound, i.e. methane. It has to be assumed that the four valence electrons are equivalent. This is source of confusion no. 8. The $2s$ and $2p$ levels differ in energy and therefore they do not seem adequate for the formation of such a methane molecule. The decision to use the average energy value seems an ad hoc solution.

SC 9. The last source of confusion is the most important in our view. The structure of the atom described in the previous sections is not consistent with the description of molecule formation. The crucial concept for bonding appears to be the bonding electron pair (cf. the quotation from Section 10.5 of Hoofdstuk 10). However, this pair differs from the electron pair in the previous sections. It is now situated as an electron cloud *between* the nuclei and holds them together, contrary to the electron cloud *around* the nucleus in the free atom. Furthermore, the lower energy of the combination of two electrons is not explained and not linked to experimental data, such as ionisation energies or spectral lines.

The great discrepancy between the descriptions of atoms, including the images evoked, before and after bonding caused us to call this inconsistency: the gap.

There are more indications for this gap: once the formation of the molecules is described the energy levels are mentioned only once or twice. Instead, bonding is governed by the octet rule or rule of eight. This rule is used in assignments and has to be applied also in the cases of mesomerism and reaction mechanisms. Numbers of electrons, not energies of electrons are decisive. How bonding should be described if the rule of eight does not apply, is not discussed in Hoofdstuk 10.

1.3 Analysis of the Sources of Confusion

In this section I report on a further analysis of the sources of confusion as part of the revision of Hoofdstuk 10 project.

A teacher working with a schoolbook needs a coherent presentation of the chemical concepts that are to be taught and learnt. Therefore, we analyzed the inconsistencies to find out what could be done to improve the coherence.

First, I relate the sources of confusion to each other and to the statement that the structure of the electron cloud determines chemical properties. Then, I focus on working with models; and thirdly, I discuss macro-micro relationships, i.e. relations between macroscopic phenomena and microscopic particles (cf. Lijnse, Licht, De Vos and Waarlo, 1990).

As a result of the analysis, three descriptions can be given of the gap, which is the main source of confusion. These will be presented below.

The gap and the structure of the electron cloud. The intended coherence of chemical concepts is expressed in the sentence on the importance of the electron cloud (see quotation from Section 10.2 of Hoofdstuk 10 on the electron cloud). This states that examination of the structure of the electron cloud is worthwhile because the electron cloud determines the chemical properties of elements.

Apparently, the structure of the electron cloud is considered to be sufficiently known when the electron configurations are drawn up. This drawing up is to be done by using concepts such as ionisation energy, energy level, distance and spin, together with information on specific elements from the Periodic Table. Furthermore, in Hoofdstuk 10, the sequence of the sections on atomic structure (10.2-10.4) and the section on the formation of chemical bonds (10.5) suggests a logical connection between the sections and implies that students need to be familiar with atomic structure before the formation of molecules can be described.

In this part of our analysis, the sources of confusion will therefore be considered in relation to each other, to the structure of the electron cloud and to the assumption of a logical sequence of sections in Hoofdstuk 10.

The first two sources of confusion, SC 1 and SC 2, concern the development of energy levels from ionisation energies and the representation of both concepts in diagrams made by students and in figures in Hoofdstuk 10. The text accompanying the figures is not effective in making clear the relation between the two concepts, ionisation energy and energy level, and between the meanings of the various figures. The point of both is that energy levels are assumed to be informative on the structure of the electron cloud (and hence, about the chemical properties of the elements).

The choice of the reference point is confusing for SC 2 as well as for SC 3. The direction of counting is different for the ionisation energy and for the energy level of the

first electron in subsequent atomic species in SC 2. The direction is also reversed in the figures of the energy levels and the distance to the nucleus as discussed in SC 3. The interpretation in terms of the electron cloud is that energy levels appear to have the nucleus of an atom as reference point.

The sources of confusion SC 3 and SC 4 are related to the intention to give a description of a *spatial* structure of the electron cloud. This is to be achieved by combining energy levels and distances from the nucleus with the help of Coulomb's law. If only electrostatic energy is taken into account, this might be valid. However, as I have pointed out in the previous section, this law is no help when the spin is introduced. The concept of spin is supposedly necessary to distribute the electrons in pairs over energy levels. I remarked earlier that SC 5 is the apparent inconsistency of two negatively charged electrons staying together. A similar confusion is apparent when in the formation of a molecule the (shared) electron pair is attributed a meaning of a bonding electron pair holding two positively charged nuclei together.

Complications of using Coulomb's law are related to SC 3, SC 4 and also SC 6 as they have the common feature of using and mixing 'energy level' and 'distance from the nucleus'. It might be expected that, in this way, energy level description of the electron cloud will take on the meaning of distance in the structure of the electron cloud and that 'level' might *become* 'distance'. If the figure of the hydrogen atom with the segments of concentric circles gives reason to mention the shells in Bohr's model of an atom, a third meaning can be added: energy level ~ distance ~ shell.

With regard to SC 7: the valence electrons are an important concept for chemical properties, i.e. for chemistry. However, this concept is introduced in the section on the structure of the atom without a proper legitimization and, therefore, rather prematurely. The role of the valence electrons in the structure of the electron cloud in relation to the filling up procedure of energy levels remains unclear.

The sequence of the sections suggests that the formation of a molecule should *follow* from the structure of the atoms and that the electron cloud is a *preparatory condition* for bond formation. Mentioning atoms with a partially filled *p* level in section 10.4 is an indication that the structure of the electron cloud might be used for the formation of molecules in the next section of Hoofdstuk 10. However, this section starts not with the filling up of a *p* level, but with the bond of a hydrogen molecule, and therefore with what might be considered as a bond between partially filled *s* levels.

Furthermore, the structure of the electron cloud is hardly used for the description of bonding, or when it is used, it has been adapted first for instance in the equivalency of the four bonds in a methane molecule, as described in SC 8.

The main source of confusion, the 'gap', may be caused by the fact that the sequence in which the concepts are presented in the consecutive sections is not as logical as intended.

The gap, SC 9, is an indication that the structure of the electron cloud developed in the subsequent sections is not applicable for the description of the formation of a molecule.

The gap and working with models. With regard to the aspect of working with models, the nature and function of models are not mentioned in the introductory section of Hoofdstuk 10 when the role of theories is very briefly discussed. Nor is special attention paid to the introduction of models or to working with models. The word 'model' can be found in Hoofdstuk 10 in a few places: when it is said that the energy model has to be refined, when Bohr's model of the atom is mentioned, and when a model of the structure of the electron cloud around the nucleus is being developed. The description of the structure of atoms and molecules in terms of energy level, distance from the nucleus, electron cloud, etc. takes place without reference to model features or hypothetical aspects of models and theories.

The filling-up procedure, the so-called Aufbau principle, for the electron configurations might be regarded as a step by step construction not of the structure itself but of a *model* of the structure of the electron clouds of various atoms. The "energy model that has to be refined" referred to earlier can be seen as a first draft of a model of the structure of the electron cloud. As can be gathered from the description of SC 3, this refinement implies the acceptance of the concept of 'distance from the nucleus' for a structural conception of the electron cloud. The energy model has been refined by extending it to include the distances.

However, changing of the point of reference suggests that another model of an atom is constructed, a distance model.

In SC 4, Bohr's model of the atom is given as a model in which a combination of energy and distance is possible. In Hoofdstuk 10, this model is restricted to the hydrogen atom. The introduction seems to imply that this model can be used for the structure of the electron cloud of other atomic species. However, constructing the model of the structure of the electron cloud in this way is confusing because the meaning of an energy level representing an amount of energy is extended to depicting a distance to the nucleus. This confusion may be interpreted as a mixing up of the energy level model and the distance model.

SC 6, the $4s$ - $3d$ dilemma, can also be interpreted as an example of this confusion. The $4s$ level is lower than the $3d$ level according to the filling up procedure of the energy model. But, when electrons are removed during ionisation, the electron in the $4s$ level, the one furthest away, goes first. The electrons in the $4s$ level had to be on the periphery of the atom in accordance with the distance model.

The comment in Section 10.4 of Hoofdstuk 10 is important in that here assumptions are mentioned to be taken into account for the different position of energy levels in 'free' atoms and in atoms in molecules.

This might imply that two models are under consideration, *one of free atoms and one of atoms bonded in molecules*.

In Hoofdstuk 10, however, the model of the free atom seems no adequate preparation for the model of the bonded atom in a molecule. The model of the free atom concerns primarily electrons and their energy levels. For the model of the bonded atom, the positions of the electrons with regard to the nuclei and of the nuclei to each other are important. The sources of confusion SC 7, valence electrons, and SC 8, the tetravalency of the carbon atom are related to the models with bonded atoms.

The gap, SC 9, can be described as a result of using two different models, viz., a model of a free atom and a model of a bonded atom.

The gap and macro-micro relationships. The third aspect to be discussed regards macro-micro relationships, a distinction between macroscopic phenomena and microscopic particles and the relation between these two. I already mentioned that Hoofdstuk 10 is a chapter on theoretical concepts with the apparent objective of extending students' knowledge of atoms, molecules and bonding. Only a few references are made to macroscopic phenomena and no experiments are included in Hoofdstuk 10. Yet in some cases, the experimental basis of the data is mentioned, such as the experiment of Franck and Hertz in the case of ionisation energies, the crystallographic measurements for the atomic radii and spectra for wave length and energy calculations with light. These experiments involve physical measurements and can be seen as belonging to the domain of physics. No specific chemical experiments are mentioned: i.e. no examples of reactions are given in the three sections on atomic structure preceding the gap. Reference is made to chemical properties when the periodic table is discussed and when the filling-up procedure of energy levels of the atoms starting with scandium is to be completed by comparing the electron configuration to the place of the elements in the Periodic Table.

With regard to the gap we concluded that Hoofdstuk 10 offers a physical introduction to chemical bonding. The model of the free atom explains physical phenomena and was designed for that purpose.

1.4 Recommendations for Revision

After the analysis of the sources of confusion, we must turn to the question of how to enhance coherence and how to prevent the inconsistencies in a revision of Hoofdstuk 10. These questions must be considered from the perspective of the position and the function of Hoofdstuk 10 in the existing method. The proposed improvements take into account the conclusions of the previous section with regard to the three descriptions of the gap. I will also discuss what we have recommended for each of the subsequent sources of confusion as a result of the project.

For the revision of Hoofdstuk 10, we had to bear in mind that this chapter was part of a series of textbooks used in many schools in the Netherlands. Therefore, the revised version had to continue to comply with the requirements of the Netherlands exam syllabus (Eindexamenprogramma, 1984) and had to fit into the prevailing curriculum (Leerplan, 1984). In addition, the version had to comply with the conceptions of the publisher and the Gebruikersredactie regarding the working methods and presentation of content, to ensure that the revised chapter would be acceptable to the teachers using the method. The improvements we proposed proved to be applicable within the framework of the examination programme and the conceptions of the method: draft versions of the revised chapter were tested in classes. We also presented the results of our analysis to teachers on various occasions.

We took measures to lessen the effect of the 'gap'. We maintained the sequence of the structure of the atom followed by the formation of molecules, as well as the physical nature of the introduction. However, more emphasis is laid on the importance of knowing more about the structure of atoms.

Although the proposal does not include laboratory experiments, experimental conditions and results are presented in more detail and it is suggested that teachers demonstrate the experiment of Franck and Hertz (during physics lessons).

The most important aspect of the proposed changes is the strong emphasis we laid upon model features of descriptions of atoms. We tried to give this shape by presenting the development of models in historical sequence and by pointing out the necessity of changing, adapting or even rejecting a model when new experimental results require this.

We decided to explicitly emphasize the 'gap' by *presenting two incompatible models next to each other* and we provided opportunities to discuss the merits of each of these models.

The first model describes a free atom and is called a model using distances or a *distance model*. This model uses, in a more consistent manner, ionisation energy values to develop a notion of distance. So that, in fact, this is a consistent distance-energy model. The second model is designed for an atom bonded in a molecule. The name *charge-cloud model* is used for this model.

I describe briefly how the distance model is developed in the proposal. More information can be found in Van Hoeve-Brouwer, Vroemen and De Vos (1993).

We start from *ionisation energies* and work first towards corresponding (*relative*) *distances from electrons to the nucleus*, using Coulomb's law in the energy formulation and assuming the energy to be electrostatic in nature. This leads to a model of a spatial structure of the atom. Only then energy levels are introduced as related to distances within this model. Each distance between an electron and the centre of the atom in the model corresponds to an energy level.

As is the case in Hoofdstuk 10, we start from the experimental values of ionisation energy of the sodium atom. However, in our approach, each value of an ionisation energy is divided by the number of the respective electron instead of taking the logarithm of that value. The results are presented in the following table:

number of the electron:	1	2	3	4	5	6	7	8	9	10	11
ionisation energy (eV)	5.14	47.29	71.8	98.9	139	172	208	264	300	1465	1646
quotient	5.14	23.65	23.9	24.7	27.8	28.7	29.7	33.0	33.3	146.5	149.6

In the resulting row of quotients the same pattern appears as in the plot of the logarithms, that is, a division roughly into three groups of 1, 8 and 2 electrons respectively. The difference is that we can now attribute a physical meaning to the quotient values by using a simplified model in which the net positive charge of the ion left behind by an electron is supposed to be situated in the nucleus. Coulomb's law is expressed as

$$E = f Q_1 Q_2 / r$$

for calculations within this model. With the help of these assumptions and calculations we find a measure for the relative distance of each electron to the nucleus. The pattern that will appear is quite similar to the pattern of Figure 1.1. The advantage is that this procedure is applicable to *all electrons of other atomic species* if the ionisation energies of these atoms are known. It is therefore not necessary to introduce Figure 1.1 which is only valid for the *first electrons of subsequent atomic species*. Another advantage is that small differences in electron-nucleus distances, e.g., between electron 10 and 11 of sodium, can now be attributed to imperfections in the model. It can be assumed that these two electrons are at the same distance and, later on, that they occupy the same energy level.

By using the distances between the electrons and the nucleus, the model chosen produces a depiction of the atom in which the electrons and the nucleus are point-like objects. This cannot explain bond directions nor does it offer a model of electrons in many atom systems. Consequently, the distance model is not a model appropriate for bridging the gap.

The model we proposed for the other side of the gap, the charge-cloud model, is designed for atoms bonded in molecules. We start with the methane molecule, CH₄. It is pointed out that this molecule is stable and that the spatial orientation of all four C-H bonds is equivalent. We refer to Van 't Hoff's work on the number of isomers of chlorinated methane and on optical activity to illustrate this. The depiction of electrons around the nucleus shows a space around the nucleus with domains where electrons can

be found. The electrons are seen as charge (sub)clouds taking up parts of the space, each of the electrons involved being assigned to a (sub)cloud. Bonding with a shared electron pair between two atoms is described as a partial overlap of two (sub)clouds with a domain available for the two electrons.

To let the students gain experience with some aspects of models we included a separate section on the model features of the various descriptions and on working with models. We present assignments on the choice of a model to explain phenomena. Two incompatible models were introduced to underline the differences between the model features of the two descriptions.

In the proposal for revision the subsequent sources of confusion are taken care of as follows.

In view of the sources of confusion, SC 1 and 2, we paid continuous attention to the use of language and the design of diagrams in order to improve on the phrasing in the text and on the relation between text and illustrations.

The introduction of the distance model in the proposal is intended to avoid the difficulties connected with SC 3 and 4. By choosing a different sequence it is possible to develop a structure for the electron cloud, i.e., distance notions coming before energy levels, instead of the other way round as in Hoofdstuk 10.

We did not suggest a solution for SC 5, the introduction of the spin. The spin is *postulated* and used in formulating rules for the filling-up procedure of energy levels.

The *4s-3d* dilemma, SC 6, also stays unsolved but it is less pronounced, because, in general, more emphasis is laid on the relationship between the distribution of the electrons and the position of an element in the Periodic Table. The filling-up procedure with a sequence of energy levels remained restricted to the first twenty atomic species.

The valence electrons, SC 7, are still mentioned in the part on the free atoms but just before the section on the molecules begins, and therefore less prematurely.

The improvement proposed for SC 8, the tetravalency of a carbon atom, is included in the design of the charge cloud model. No attempt is made to link this with the distance model.

Together with the distance model, the charge cloud model constitutes a multi-model approach, which is the central idea in our suggestion for explicitly dealing with SC 9, the gap.

1.5 Results and Questions for Investigation

In this section I will discuss the outcomes of the small scale project 'Revision of Hoofdstuk 10'. The outcomes are twofold: first, the results of the project are a concept text for the third edition of *Chemie*, and a recognition of the gap by teachers and also by

students; and, secondly, the project was to be continued in a PhD research project on chemical bonding.

The first result of the small scale project is a revised text for Hoofdstuk 10. The parts of this text relevant to the structure of atoms and the formation of molecules are described in the previous section of this thesis. The Gebruikersredactie incorporated most of the proposed text in the third edition of CHEMIE published in 1993 (Pieren, Scholte, Smilde, Vroemen and Davids, 1993, p.9-44). The content and the design of the final text in the third edition is the responsibility of the Gebruikersredactie.

During the project we discussed our findings with several other teachers on a number of occasions. One of these discussions took place during the 'Gebruikersdag', an annual meeting of teachers using the CHEMIE series organized by the Gebruikersredactie and the publisher, Wolters-Noordhoff. On these occasions, it became clear that the inconsistencies we had found, especially the gap, were recognized by most teachers. Some teachers mentioned that they present additional material on hybridization to their students and suggested including the concept of hybridization in the revised text. This suggestion was interpreted by us as an attempt to bridge the gap, and as an indication of a preference for a more chemical approach.

The relation of the content of Hoofdstuk 10 to the model nature of descriptions of atomic structure and chemical bonding in molecules also came up for discussion. It was seen as an advantage that students should experience working with models and in this way get an idea of the use and usefulness of models. According to teachers, working with models should be related to the experience with models acquired by students in earlier years, such as Dalton's and Rutherford's models of atoms.

We tried out versions of the revised text in classrooms. During one of the lessons students were engaged in answering a question on the applicability of models. The following students' discussion on which model to choose was recorded on a tape recorder.

Se Distance model, that is with those different energy levels, isn't it?

St What can you explain with this?

Se Yes, this.

Sd Ionisation energy.

St Yes, I think so.

Sv The emission of light.

Sv But that's not chemistry, you know, that's physics.

In our interpretation of this discussion, it indicates that the gap is experienced and recognized by students.

The second outcome of the small scale project is the continuation of the project in a PhD research project entitled "An Educational Structure of Chemical Bonding".

As I mentioned in the previous section the proposal for the revised text contained no solution to all sources of confusion and several difficulties were left unaddressed. The sequence in which the topics were presented, the model of the free atom followed by the model of the bonded atom remained unaltered, as well as the use of physical theory to prepare the way before introducing the formation of a molecule. Besides, it was concluded that more attention should be paid to working with models in teaching and learning.

One of the reasons for not going into these difficulties was the limited amount of time available. The activities of the small scale project were spread over a couple of years, and had to be carried out in addition to daily teaching work and partly on a voluntary basis. Therefore, the opportunities to look for alternative topics and/or approaches were limited.

Another reason was that proposed revisions had to fit into the framework of the prescribed curriculum as interpreted in Hoofdstuk 10. This framework contains the assumption that the electron cloud determines the chemical properties of the element. In a PhD research project it is possible to bring the framework up for discussion and to question the validity of assumptions regarding the electron cloud or the sequence from free atom to molecule.

The PhD research project started in 1990 and had two aims:

(i) to perform an educational analysis of chemical bonding and related concepts;

In an *educational analysis* various meanings of chemical concepts, including chemical procedures, are analyzed in their relationship to each other and their relevance for teaching and learning chemistry. The meanings can be found in the chemistry practice of chemists, teachers, students, historians, philosophers, authors and others.

(ii) to develop an educational structure for chemical bonding.

An *educational structure* is worked out through educational analysis and educational experiments. Chemical concepts and how they are related to each other are described in this educational structure through what emerges from the educational experiments with regard to the teachability and the learnability of these concepts.

I will give an overview of the following chapters of this thesis in relation to the two aims of the research project on chemical bonding.

ad (i) The objective of the educational analysis of chemical bonding was to go more deeply into the meanings and relevance of chemical concepts, and how they are interconnected. The results of the small scale project were used as a starting point for this thesis.

The following questions will be addressed in the educational analysis:

- Can chemical bonding be explained starting from the structure of the electron cloud as described in Hoofdstuk 10?

- What explanations of chemical bonding are accepted by contemporary chemists and what is the role of physical theories in such explanations?

These questions will be discussed in Chapter 2.

In explanations of chemical bonding models of atoms and molecules are used. The need to understand models and, consequently, the acceptance and use of models is relevant for teaching and learning chemical bonding.

Therefore a question on aspects of models was formulated:

- How can students acquire insight into models and working with models?

This question is addressed in Chapter 3.

A preference for a more chemical approach to chemical bonding is incorporated in the question:

- Can chemical bonding be approached from a more chemical point of view in secondary education?

I will explore a route to such an approach in Chapter 4. In this chapter I will also go into the criteria to be used when designing an educational text on chemical bonding.

ad (ii) Based on the results of the small scale project and the educational analysis, an experimental teaching unit was designed in which teaching and learning aspects related to the above questions on models and a chemical approach were incorporated.

The development of an educational structure for chemical bonding took place in the framework of an educational experiment.

The question is:

- Can students gain an understanding of the relativity of models in the context of chemical bonding?

How the chemical concepts and further criteria for the design were incorporated into the educational text is discussed in Chapter 5, in which the results of the first experiments in the classroom are also reported.

For a second educational experiment, a revised version of the educational text was written. Chapter 6 gives the reasons behind the adjustments of the educational text for the second round of testing and reports on the results of the adjustments and testing.

To conclude, a tentative educational structure for chemical bonding will be presented.

2 Reflections on Chemical Bonding

The educational analysis of chemical bonding starts in 'Hoofdstuk 10', a chapter on atomic structure and formation of molecules in a chemistry textbook. In the previous chapter of this thesis I gave an analysis of Hoofdstuk 10. In this chapter, I address the first two research questions by taking a closer look at the inconsistencies, or sources of confusion (SC's) as I have called them.

The major inconsistency is the *gap* between the model of free atoms and the model of bonded atoms. Free atoms might be regarded as belonging to the physics context whereas the bonded atoms belong to the chemistry context. I will discuss whether approaching the topic from the context of physics could lead to confusion when trying to understand bonding in a chemistry context. The first question is whether chemical bonding can be explained by starting from the structure of the electron cloud as described in Hoofdstuk 10?

The gap may be a result of the design of a specific school text, or it may exist in other textbooks as well. Another possibility is that the gap is actually present in chemistry as a science. This is not unlikely, since the content of the entire chemistry curriculum on chemical bonding is derived from chemistry as a scientific discipline. The second question to be examined is: What explanations of chemical bonding are accepted by contemporary chemists and what is the role of physical theories in such explanations? In other words, I need to look further than school chemistry alone to find an explanation for the gap and a solution for bridging the gap.

To begin with, I distinguish between the chemistry context and the physics context as mentioned above, I discuss some aspects of bonding and types of bond and I classify the sources of confusion as belonging to one or the other context in Section 2.1. Then I look into possible reasons for the approach of chemical bonding from a physics context, dealing in Section 2.2 with those reasons which are associated with the educational setting and, then in Section 2.3, with reasons associated with relationships between chemical and physical theories. In the last section of this chapter, 2.4, two combinations of chemistry and physics contexts are discussed.

2.1 Source of Confusion: Chemistry Context or Physics Context

In the previous chapter it was concluded that Hoofdstuk 10 presents a *physical* introduction in order to describe and explain *chemical* bonding. The description of a molecule with bonded atoms belongs to a chemistry context and the description of free atoms belongs to a physics context because of the way the structure of the electron cloud is presented. I examine the role of the electron cloud in order to back up these assertions and to characterize the two contexts.

It is explicitly stated in Hoofdstuk 10 that the electron cloud determines the chemical properties of an element and that therefore it makes sense to investigate the structure of the cloud (see Hoofdstuk 10 (10.2) quoted in Section 1.1). However, in Hoofdstuk 10 a gap is visible between the description of a free atom and that of an atom bonded in a molecule. This discrepancy led to the question: *Can chemical bonding be explained by starting from the structure of the electron cloud as described in Hoofdstuk 10?*

To find out which parts of Hoofdstuk 10 on the structure of the electron cloud in a free atom are used to describe chemical bonding, I quote the description of a chemical bond in Hoofdstuk 10:

"An H atom has 1 electron in the 1s-level. This also applies to the other H atom with which a molecule H_2 must be formed. Both electrons form an electron pair which lies as a shared electron cloud between the two positive nuclei. This shared electron pair has a lower energy value than the sum of the energy of the individual electrons." (...)

"The electron pair holds the two nuclei together. The electrons are a *bonding electron pair*." (CHEMIE 5/6V, 1985, p.284; italics in the original text)¹

Two aspects of the electron cloud are used to describe the formation of a bonding pair in this quotation, viz., the aspect "lower energy" and the aspect "holding together" in a spatial sense.

First, I discuss the statement about the shared electron pair which is said to have *lower energy*. The energy decrease could be seen as a result of the formation of the pair or as a result of the sharing of this pair by the nuclei. Nothing is mentioned, however, about lower energy of the molecule *as a whole* compared to the energy of the two separate atoms. I focus, therefore, on what is said about the electron pair. In the previous text in Hoofdstuk 10 no indications can be found as to why an electron pair should have less energy than the sum of the energy of the two separate electrons. Mentioning lower energy suggests that data from a physics context will be used to explain this. However, no experimental data, such as spectra for instance, are given which could indicate that in a hydrogen molecule the two electrons are on a lower energy level. There is not even any mention of ionisation energy measurements although they were used in the previous text to introduce energy levels.

The source of confusion SC 5 relates the occurrence of two electrons as a pair to spin as a property attributed to each electron. From the point of view of the physics context,

¹ "Een H atoom heeft 1 elektron in het 1s-niveau. Dit geldt ook voor het andere H atoom, waarmee een molecuul H_2 moet worden gevormd. De beide elektronen vormen nu een elektronenpaar dat als een gemeenschappelijke elektronenwolk tussen de beide positieve kernen ligt. Dit gemeenschappelijk elektronenpaar heeft een lagere energie dan de afzonderlijke atomen tezamen." (...)

"Het elektronenpaar houdt de beide kernen bij elkaar. De elektronen zijn hier een *bindend elektronenpaar*." (CHEMIE 5/6V, 1985, p.284)

this spin concept is linked to interpretations of spectra. However, in the chemistry context no experimental proof is given about the formation of an electron pair to be described on the basis of spin. In Hoofdstuk 10 nothing is said about the lower energy of two paired electrons with opposite spin. *The lower energy of a bonding electron pair is apparently not a consequence of the structure of the electron cloud.*

For the second aspect, that of "holding together", I refer to the statement in the quotation on the position of the electron pair as a shared electron cloud. In previous paragraphs in Hoofdstuk 10 an electron cloud is always situated *around* a nucleus; in the quotation, a cloud is more specifically said to be *between* two nuclei. This is contrary to the model of a free atom in which an electron is either part of the electron cloud around the nucleus or it is not part of the atom at all. A spatial notion has been introduced which in the case of the hydrogen molecule corresponds to distance (between two nuclei).

From this discussion of the two aspects, "lower energy" and "holding together", I conclude that in Hoofdstuk 10, knowledge of the structure of the electron cloud (physics context) is not used to explain the formation of a chemical bond in a hydrogen molecule (chemistry context).

The way energy is introduced with ionisation energies and energy levels in the electron cloud of a free atom is useful for explaining spectra, i.e. in a physics context. The spatial notion, on the other hand, is relevant for molecules in which atoms occupy specific positions with respect to each other. This I regard as belonging to the chemistry context.

It is mentioned in the quotation on the formation of a hydrogen molecule that the electron of the free hydrogen atom is in the 1s level. This is in agreement with previous statements on energy levels. In the following quotation, the electrons in the highest energy level are called valence electrons:

"Only the electrons in the highest energy level have any significance for the chemical properties of an element. These are the only electrons that can interact with the electrons of the other atoms, or are released during the formation of a positive ion. It is therefore usually not necessary to write down the complete electronic configuration of an atom. The electrons in the highest energy level are called valence electrons." (CHEMIE 5/6V, 1985, p.279-280)²

At this point in Hoofdstuk 10, I consider this statement premature and therefore I call it a source of confusion, SC 7. But where it could have been useful, i.e. in the description of the formation of a molecule H₂, it is not mentioned that the electron in the 1s level of the hydrogen atom is a valence electron that can "interact" with another

² "Voor de chemische eigenschappen van een element zijn alleen de elektronen in het hoogste energieniveau interessant. Alleen deze kunnen met de elektronen van andere atomen iets doen of alleen deze kunnen bij de vorming van een positief ion afgestaan worden. Daarom is het meestal niet nodig om de volledige elektronenconfiguratie van een atoom op te schrijven. De elektronen in het hoogste energie niveau noemt men valentie-elektronen." (CHEMIE 5/6V, 1985, p.279-280)

electron. This would imply the use of a 'rule of two' for valence electrons. In the text following the description of a hydrogen molecule, the formation of shared electron pairs is governed by the number of eight electrons in the "highest energy level", or by the octet rule which I see as belonging to the chemistry context.

I will now discuss two types of bond, the covalent bond and the ionic bond, in relation to the sources of confusion. With regard to chemical bonding, the formation of a shared electron pair pertains to the formation of a covalent bond. The above-mentioned quotation on the valence electrons provides information on the possibility of another bond type, i.e. an ionic bond. The valence electrons in the highest energy level have two possibilities: they can "interact with electrons" of other atoms or they can be released during the formation of a positive ion. Only a few electrons will be expelled, since the values of successive ionisation energies increase considerably. Therefore, low values of positive electrovalency can be explained. The formation of negative ions is, however, not made plausible. Interacting with electrons of other atoms might be interpreted as a possible electron transfer. Consequently, rules should be provided indicating where the transferred electrons could be placed. It might be concluded from the filling-up procedure of the subsequent atomic species that free places in the highest energy level are relevant in this respect. However, in Hoofdstuk 10, it is not the free atom description but information from the Periodic Table which is used to determine the number and location of these free places, which in turn is used to describe the formation of negative ions with low values of negative electrovalency.

From the description of the free atom, ionisation energy, energy level and distance might be useful concepts describing positive electrovalency, but not negative electrovalency, and therefore not the ionic bond.

The statement on the valence electrons as "interacting with electrons of other atoms" might have more relevance for the covalent bond. But then, I presume that "highest" in the "highest energy level" does not indicate a specific energy value, but that it refers to the periphery of the atom and therefore to the *position* of the valence electrons. The position of the electrons in a covalent bond is between the nuclei. As mentioned before with regard to the electron cloud, the position of electrons between nuclei is not related to distance in the free atom, and therefore not to the physical introduction. Position is a relevant factor in the discussion of the valency of a carbon atom in a methane molecule, not only with regard to the position of valence electrons between the nuclei of the carbon atom and the hydrogen atoms but also regarding the orientation of the resulting bonds in space.

Equivalent carbon bonds in a methane molecule (SC 8) involve not only stoichiometric and energetic equivalence but also geometrical equivalence.

With regard to differences in contexts, on the bonded atom side of the gap in Hoofdstuk 10, descriptions are given of atoms with spatially oriented, equivalent covalent bonds, which are meant to be used for describing, explaining and predicting chemical properties. Valence electrons and equivalence of bonds in a methane molecule belong to a context where atoms are in a bonded situation: the context of chemistry. In contrast to this, the description of the electron cloud of a free atom given before the gap uses energy levels to explain and predict spectra. Bohr's model of the atom illustrates this. Energy levels, spectra and ionisation energies with regard to free atoms belong to a physics context.

I classify the sources of confusion about ionisation energies and energy levels (SC 1, 2, 3, 4 and SC 6) as belonging to the physics context. The sources of confusion concerning valence electrons and valency (SC 7 and 8) belong to the chemistry context. SC 5 is a special case: in explanations of spectra, spin can be attributed to the physics context. When spin is used to make the occurrence of electrons in pairs plausible, it can be seen as belonging to the chemistry context.

I described the source of confusion SC 9, the gap, as the difference between a model of a free atom and a model of a bonded atom. The gap is of a more general nature than the other sources of confusion. Therefore I add the following to the descriptions of the gap (cf. Section 1.3): *The gap can be regarded as the difference between a chemistry context and a physics context.*

It seems that, at least in Hoofdstuk 10, the concepts and procedures of the physics context fail to prepare the way for concepts and procedures in the chemistry context. This may be due to imperfections in this text, but since the physical introduction to chemical bonding, and the gap, can also be observed in other textbooks, it has to be seen in a wider perspective. Examining how atomic structure and chemical bonding are presented in three other secondary school textbooks in the Netherlands reveals that two of these textbooks deal with these topics in the same order as Hoofdstuk 10, i.e. *Chemie in theorie en praktijk 3V* (Van Keulen, Van Gastel and Smit, 1984) and *Chemie Overal 6V* (Reiding, Franken and Kabel-Van den Brand, 1987). In the third textbook, this is also the case, although this book, which is intended for Year 11, presents a simpler version of atomic structure (*Scheikunde voor voortgezet onderwijs 2V*: Van Antwerpen, Arentsen, Bouma, Groen, Hamann, Van 't Land, Schuijl and Termaat, 1985). In the part of this series for Year 13, a more detailed description is given of the electron cloud in relation to the Periodic Table, but this is not followed by a section on chemical bonding (*Scheikunde voor voortgezet onderwijs 4V*: Van Antwerpen, Arentsen, Bouma, Groen, Hamann, Van 't Land, Schuijl and Termaat, 1987).

As to the question of whether these three textbooks can explain chemical bonding on the basis of the structure of the electron cloud, the answer turns out to be negative (cf. Van Hoeve-Brouwer and Van der Linden, 1991).

The next question that arises is whether, in chemical education, chemical bonding should be approached from a physics context. I relate this question to the assumption that fundamental physical theories are *required* for teaching chemical bonding. This will be discussed in the next section.

2.2 The Role of Quantum Mechanics

In this section I discuss the assumption that fundamental physical theories, and quantum mechanics in particular, are a prerequisite for teaching and learning chemical bonding. Next, some problems associated with this approach are discussed, followed by some solutions that have been proposed.

The preference for a physical introduction to chemical bonding is not found in the exam syllabus for secondary education in chemistry (Eindexamenprogramma, 1984). The topics for the chemistry examination in this document include concepts regarding atomic structure and chemical bonding, but no sequential order is prescribed. Likewise the curriculum 'het Leerplan voor rijksscholen' (1984), in force at the time of the second edition of CHEMIE, does not prescribe an explicit sequential treatment, but a sequence seems implicit in the listing of the concepts to be taught.

The apparent preference for the sequence must have had its origins elsewhere, as might be concluded from indications for a movement which advocated this approach. This was discussed in a special issue of the Netherlands science teachers' journal FARADAY (1975) and in a special issue of CHEMISCH MAGAZINE of the Netherlands Royal Chemical Society (1980), both devoted to the teaching of chemical bonding in secondary education.

Kollaard (1980) discusses preconditions for educational reconstruction of subject matter. With respect to a theory on chemical bonding he argues:

"The basic assumptions must be consistent with well-known, well-founded and generally accepted physical principles." (Kollaard, 1980, p.299)³

Aerts and Van Duijnen (1980, p.308) agree with Kollaard on the importance of fundamental, theoretical physical aspects.

Kollaard (1970) and Van Duijnen and Höhle (1975, p.2-18) argue explicitly, both in above-mentioned and other publications, that since physical principles underlie chemistry, these should be included in chemistry education:

"Chemistry teaching must seriously begin to appreciate the fact that the theoretical basis of chemistry lies in physics." (Kollaard, 1970, p.138)

These authors appear to be of the opinion that the chemistry curriculum in secondary education should reflect scientific developments. Furthermore, the introduction to

³ "Die uitgangspunten moeten voorts consistent zijn met goed bekende, goed gefundeerde en algemeen geaccepteerde fysieke principes." (Kollaard, 1980, p.299)

physics should be adequate for secondary education, but also give a logical foundation for the more sophisticated theories such as quantum mechanics. They propose adapted introductions for that purpose (Van Duijnen and Höhle, 1975, p.2-18; Van Duijnen and Aerts, 1980, p.302-306; Kollaard, 1973). The authors feel that these adaptations are justified in view of the complex mathematics involved, among other things. But they do not doubt that it is possible to explain chemical bonding in secondary education in a scientific sense, from physical 'first principles'.

The textbooks that became available in the Netherlands in the nineteen eighties have not fully adopted these new introductions. The textbooks do refer, in more or less detail, to quantum mechanics as a fundamental theory. The textbooks mention the theory as something that will be presented at the next, higher, level of education (which in this case is the university) and discuss some aspects of quantum theories. In Hoofdstuk 10 these aspects are covered by an optional section which gives a short summary of the historical developments from Bohr's model of the atom to mathematical models in quantum mechanics.

It is understandable that teachers using these textbooks also refer to advanced scientific theories when students ask questions prompted by the gap or other sources of confusion. Various concepts from quantum theory or quantum chemistry might be mentioned, for instance, hybridization in the case of the equivalence of the carbon bonds in methane, and orbitals or drawings of orbitals in the case of spin, to distinguish between the electrons in a p level.

Enlisting the aid of quantum theory concepts does not bring the intended clarification for the students. Remarks commonly heard among teachers are "the theory is too difficult to be discussed at school", or, "this is something that will be dealt with in full in higher education". These remarks imply that the clarification can be achieved in more advanced scientific education. *And this means that the problems concerning the gap are passed on to chemistry education at the university.* However, students who are not pursuing their studies in chemistry will not benefit from this delayed clarification.

During the period the research reported on in this thesis was carried out, I was allowed to attend the first year course at Utrecht University on atomic structure and chemical bonding, called 'Structuur en Binding'. The students studied chapters of the prescribed textbook, PHYSICAL CHEMISTRY (Atkins, 1990). The table of contents of this textbook shows a sequential treatment of atomic structure and chemical bonding similar to Hoofdstuk 10, i.e. explicitly physics first. However, there are also significant differences as a result of the much more extensive discussion in the university textbook.

PHYSICAL CHEMISTRY starts with a discussion of failures of classical physics. Then an extended treatment of the Schrödinger equation is given, followed by descriptions of atomic structure and atomic spectra. The physical introduction is concluded with descriptions of one- and many-electron atoms. The linear combination

of atomic orbitals (LCAO) is used to explain the most simple case of bonding: the hydrogen molecule ion. In a footnote, however, the following comment is given:

"Unfortunately, this neat explanation is probably incorrect in the case of H_2^+ (at least). This is because shifting an electron away from a nucleus into the internuclear region raises its potential energy. The modern explanation is more subtle, and does not emerge from the simple LCAO treatment given here. It seems that at the same time as the electron shifts into the internuclear region, the atomic orbitals shrink. This orbital shrinkage improves the electron-nucleus attraction more than it is damaged by the migration to the internuclear region, and so there is a net lowering of potential energy. The kinetic energy of the electron is also modified, but it is dominated by the potential energy." (Atkins, 1990, p.392)

It appears that chemical bonding cannot be deduced logically from physical principles, at least not at this stage of university education.

My conclusion is that the gap exists not only in secondary education textbooks, but also in this university textbook.

The educational view of explanations for chemical bonding based on physical principles is connected with the view that the fundamental basis of chemistry lies in physics, and that physical theories are a prerequisite for approaching chemical theories. The problems with teaching and learning advanced theories such as quantum theories and their adaptation for teaching purposes are regularly the subject of discussion (cf. Sanderson, 1986, p.845-846; Ogylyvie, 1990, p.280-289; Pauling, 1992, p.519-521; Shiland, 1995, p.215-219). The unsuccessful attempts to introduce physical approaches in secondary education can be ascribed to the degree of difficulty of the subject matter. However, since even at the level of university education, success is not guaranteed, there may also be a more fundamental reason.

Of course, solutions for the problems could be looked for within the world of education, but the origins of the problems may lie beyond the world of education. There could also be a gap between chemical theories and physical theories in science, and not just in science education.

This leads to a question concerning the nature of the relationship between the context of chemistry and the context of physics in general, and the relationship between chemical phenomena and theories on the one hand, and physical phenomena and theories on the other hand.

I would like to consider this question on the basis of a reductionistic conception of science, and therefore I formulate it as follows: what is the nature of the relationship between chemical theories and physical theories when looked at from the point of view of theory reduction?

2.3 Reductionism or Pluralism

Regarding the gap between chemical and physical theories the question is whether chemical theories can or cannot be deduced from physical theories. In this section I discuss some views on reductionism (2.3.1). Subsequently, I point to the importance of molecular structure and shape in chemistry and I give an example of the adaptation of quantum mechanical theories to incorporate structural notions for use in chemistry. Finally I set forth a view on the pluralism of theories (2.3.2).

2.3.1 *Reductionism, strong or weak*

The statement that chemistry is part of physics reflects a reductionistic conception of science. This conception implies that scientific disciplines are sequentially interrelated and can be ordered according to the relationship between their research objectives. A so-called reduction ladder can be used to describe a view on reductionism. Eventually, in this view, the research objective of physics includes all others, and therefore physics must be the most fundamental discipline (Van der Vet, 1989, p.19).

A statement attributed to a radical reductionist is given by Barrow:

"The outright reductionist sees science as a straightforward hierarchy. Starting with zoology, we take the attitude that we 'understand' it when it be reduced to something more basic. In this case, that something is biology. Biology likewise is founded entirely upon chemistry; chemistry can be shown to be founded upon physics; and physics leads us back to the most elementary particle of matter. When we find them - whether they turn out to be point particles or strings - we have completed the linear chain. Thus, at each stage, the ardent reductionist claims that there is a 'why' question that always points in the same direction: inwards to the smaller scale." (Barrow, 1991, p.139).

The question in this section is: What is the nature of the relationship between chemistry and physics contexts? The answer is, according to the strict reductionistic conceptions as expressed above, that the chemistry context, i.e. chemical phenomena and chemical theories, is part of the context of physics. However, the above-mentioned claim is expressed by an "ardent reductionist", and other views of reductionism allow of a more balanced conception.

I look for such views in work of Primas (1983; 1985a,b; 1991) and Woolley (1988). Primas elaborates on reductionism in a series of two articles, entitled "Kann Chemie auf Physik reduziert werden?" (Primas, 1985a,b).

In his view:

Reductionism is the thesis that, in principle, all complex natural phenomena can be explained by the interaction of simpler subsystems. The exact sciences are especially interested in finding out whether the properties and the behaviour of matter and organisms can be explained by referring to the properties and

behaviour of their constituent parts, i.e. molecules, atoms or elementary particles. Are there any ultimate units of matter that can explain the behaviour of the material world?" (Primas, 1985a, p.109)⁴

In this 'thesis of reduction' I distinguish two steps:

Step 1: reductionism versus empirism: in this step subsystems are postulated. This means, in the case of chemistry, that a particulate nature of matter is postulated. It is important that the postulated subsystems are more "simple".

Step 2: reduction versus 'emergence': properties are attributed to the particles that allow explanations of macroscopic phenomena.

The term 'emergence' indicates that on a higher level of organisation qualitatively new properties exist, which cannot be explained purely on the basis of the lower, more fundamental layers (Primas, 1985a, p.117).

Primas distinguishes between strong and weak forms of reduction.

The reduction of a phenomenon to a theory is regarded as strong when the phenomenon can be deduced completely and without approximations from the first principles of the theory. Reduction is weak when the phenomenon is compatible with the first principles of the theory but can only be deduced by using additional assumptions and approximations (Primas, 1985a, p.109). Looking strictly at theories, strong reduction implies that "(t)he higher-level theory together with its interpretation can be deduced from the basic theory". The weak form of reduction implies that "(t)he higher level theory can be deduced from the basic theory *together* with appropriate initial and boundary conditions (Primas, 1991, p.162).

In this chapter I use the following interpretation of the two steps of the thesis of reduction. The first step entails the reduction of a phenomenon to a theory. The second step is the reduction of one theory to another, in this case, the reduction of a chemical theory to a physical theory. This step I pursue in this section.

In the above-mentioned articles Primas formulates his criticism of strong reduction of theories. He argues that "no non-trivial interdisciplinary example is known" of theory reduction in the strict sense, i.e. strong reduction (Primas, 1991, p.162).

Primas cautions against strong reduction of chemistry to physics, and in particular against reduction to quantum mechanics:

"(...) most theoretical concepts of chemistry have not yet been successfully reduced to quantum mechanics and it is an open question whether such a reduction can always be achieved." (Primas, 1983, p.309; Primas' italics)

⁴ "Reduktionismus ist die These, dass komplizierte Naturerscheinungen prinzipiell immer durch das Wechselspiel einfacher Teilsysteme erklärt werden können. In den exakten Naturwissenschaften interessiert besonders die Frage, ob die Eigenschaften und das Verhalten der Materie und der Organismen durch die Eigenschaften und das Verhalten ihrer Komponenten, Moleküle, Atome oder Elementarteilchen, erklärbar sind. Gibt es allerletzte Materieeinheiten, mit denen das Verhalten der materiellen Welt erklärt werden kann?" (Primas, 1985a, p.109).

In my interpretation of his views, *the chemistry context is not automatically a part of the physics context*. The answer to the question of whether a chemical phenomenon can be reduced to a physical theory is still open. And reduction, strong or weak, of chemical theories to physical theories could well be a questionable enterprise. This is in agreement with views brought forward by Woolley (1988, p.53).

The physics context does not cover everything needed to produce explanations in the chemistry context. The physical theory of quantum mechanics cannot lay the theoretical foundations for the whole of chemistry. Chemical phenomena are explained with concepts such as shape and structure of subsystems, i.e. molecules. These concepts do not emerge from 'first principles'. The relation between chemistry and physics is ambiguous on that point. In the words of Woolley (1988, p.53): "In fact, a correct quantum theory of matter says nothing about the structure and shape of molecules".

In the next section, I will look into the theme of structure and shape of molecules.

2.3.2 *Structure and shape: one theory or plurality of theories*

First I look into the consequences of including chemical theoretical concepts such as shape and structure in quantum theories. This will lead to a pluralistic conception of theories in science.

Primas says about shape:

"Not only clouds and crystals, but molecules, too, have a shape. However, shape is a concept that is searched for in vain among the first principles of quantum mechanics." (Primas, 1985a, p.113)⁵

On molecular structure, Primas remarks:

"The concept of molecular structure as used by chemists is compatible with the first principles of quantum mechanics, but does not follow from them (...)." (Primas, 1991, p.168)

This is a serious difficulty, *viz.*, that a molecular quantum theory may describe the characteristics of molecules in terms of energy levels and wave functions, but does not take into account structure isomerism and optical isomerism (cf. Woolley, 1988, p.57).

Chemists find this hard to accept because the spatial orientation of chemically bonded atoms is essential (most important according to Woolley, 1988, p.53) *to understand how molecules react with each other.*

The crucial notion of molecular structure is put into quantum chemistry "by hand", i.e. by introducing the Born-Oppenheimer approximation (Woolley, 1988, p.56 and p.54).

The application of quantum theories in chemistry is made possible by the Born-Oppenheimer approximation and by the enormous increase in computing capacity. As a result of the development of new generations of computers, so-called 'ab initio'

⁵ "Nicht nur Wolken und Kristalle, sondern auch Moleküle haben eine Gestalt, ein Begriff, den man unter den ersten Prinzipien der Quantenmechanik vergeblich sucht." (Primas, 1985a, p.113)

calculations are carried out on a large scale, leading to molecular modelling techniques and computational chemistry.

The procedure of the Born-Oppenheimer approximation (or approach, see Primas, 1991, p.168) can be found in numerous textbooks. One of the first descriptions is probably the following:

"By making use of the fact that the mass of every atomic nucleus is several thousand times as great as the mass of an electron, Born and Oppenheimer were able to show that an approximate solution of the complete wave equation for a molecule can be obtained by first solving the wave equation for the electrons alone, with the nuclei in a fixed configuration, and then solving a wave equation for the nuclei alone, in which a characteristic energy value of the electronic wave equation, regarded as a function of the internuclear distances, occurs as a potential function." (Pauling and Wilson, 1935, p. 259-261)

Repeating the procedure yields a value for the potential energy for each new value for the distance between the nuclei. In this manner a 'map' can be constructed of the various values of the energy of the electrons with the variation of the distance between the nuclei. This map, known as the potential energy surface, shows that for a certain position of the nuclei, related to a specific molecular (diatomic) structure, a minimum in potential energy is achieved, for example:

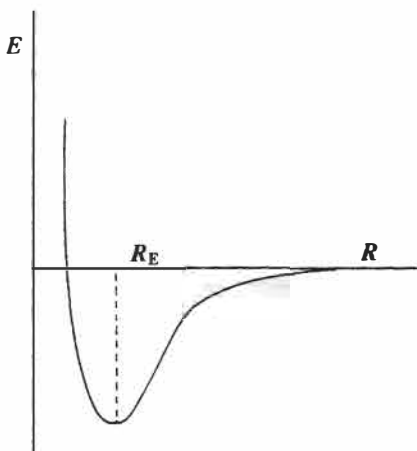


Figure 2.1 A potential energy surface

The concepts of structure and shape, which play a significant role in structural and optical isomerism in chemistry, are brought into the quantum theoretical description of a molecule by carrying out the Born-Oppenheimer approximation. *These important chemical concepts do not follow from the 'ab initio' calculations with quantum theories.*

The meaning of 'ab initio' is therefore not 'from first principles' since quantum theories are being used with additional 'boundary' conditions. In this case, a physical theory is useful in the chemistry context if chemical concepts provide the additional conditions. *Therefore, if this is an example of reduction, it is one of weak reduction.*

Primas does not reject certain aspects of reductionism (see Van Keulen, 1995, p.39). Also he cautions against taking up an anti-reductionistic position. Reductionism in the sense of a hierarchy of theories can be considered as just *one way* of relating theories to each other (albeit a very important way). Such an ordering of theories might be possible for certain (sub)theories.

However, if there is, in general, an ordering of theories in science, *this is an ordering of theories side by side*. Primas concludes that "*science is necessarily pluralistic*" (Primas, 1991, p.170; Primas' italics).

Woolley shares this opinion: "(...) it is a fundamental attribute of quantum mechanics that we never can have a single, wholly comprehensive description of a physical system. There may be several possible descriptions that may contradict each other in part." (Woolley, 1988, p.57)

From the above I conclude that there are doubts among scientists with regard to explaining chemical bonding from the 'first principles' of a physical theory. Taking the influence of chemical concepts on a physical theory into account, the conclusion might be that *the gap between the chemistry and physics contexts in science education, and possibly also in science, is a consequence of overrating the unity of the natural sciences.*

The gap might then be inherent in the relationship between chemistry and physics. Another outcome of discussions on the relation of theories is that it points to a pluralistic conception of science. Consequently, the position of chemical theories may be more autonomous than a reductionistic conception of sciences would imply.

Chemical theories and physical theories are closely related. However, having become aware of discussions among scientists I reject the reductionistic position with regard to theories, viz., that chemical theories are a part of physical theories, as the only possible approach in chemistry and, therefore, in chemistry education.

In the interpretation of reductionism I assumed in Section 2.3, that step 1 of the thesis of reduction is the reduction of a phenomenon to a theory. In the next section I will look into this and discuss whether, and if so, how phenomena from the chemistry context and physics context can be combined profitably with each other and with theoretical notions, especially with those from the chemistry context.

2.4 Pluralism: Contexts Alone and Together

In this section I continue looking into the nature of the relation between the chemistry and the physics contexts. *I will consider the role of phenomena from both contexts in establishing concepts in a theoretical framework, and whether or not the result is a fruitful combination of both contexts.*

The two concepts I want to study are on either side of the gap: *viz.* Bohr's model of the atom on the physics side, and the rule of eight generally associated with Lewis on the chemistry side (cf. Lewis, 1923, p.79). I discuss these concepts first in relation to the Periodic Table, and then in relation to the constitution and formation of the methane molecule.

I will show that the Periodic Table is a result of a fruitful combination of chemistry and physics and subsequently, that combining the contexts of chemistry and physics to describe the formation of a methane molecule is only partly successful.

2.4.1 Periodic Table and combination of contexts

The elements in the Periodic Table are arranged according to chemical and physical principles. I will mention two of these principles briefly and examine a third in more detail with regard to Bohr's model of the atom.

The first principle is attributed to Mendeleev. He arranged the elements in order of increasing atomic weight. The classification of the Table *into periods* is based, 'in principle', on chemical properties: for instance, the composition of compounds (stoichiometry), the possible valencies (selectivity) and the possibilities for reactions (reactivity). These properties have led to identifying groups of elements and, subsequently, to representing the periodicity.

The second principle is a result of Moseley's experiments, which belong to the physics context. Using X-ray analysis data, he arrived at the successive numbering of elements, and the atomic numbers. Van den Broek is also mentioned with respect to this sequencing, specifically in relation to the charge of the nucleus (Van Spronsen, 1969, p.311; see also: Joling, 1993, p.34). These experimental results from physics have not led to a change in descriptions of periodicity.

The third principle is based on experimental results, *i.e.* line spectra of gases. The name of Bohr is connected with this ordering. He designed the model of the atom that was named after him. In this model, the electron configuration of the various elements can be constructed according to the Aufbau principle. The Aufbau principle includes both the sequencing of the elements and the periodicity. Although Bohr's model of the atom is based mainly on physical principles, he not only used spectroscopic data, but referred to *chemical* properties as well. This is pointed out by several authors. For instance, Van der Vet argues that the Periodic Table accompanying Bohr's theory must have been constructed with the help of chemical information (Van de Vet, 1987, p.167). Scerri backs up this assertion (Scerri, 1993, p.51-52).

As an illustration of the relevance of chemical phenomena for the Periodic Table, I will add the example of the connection between periodicity and a fixed number of seven or eight electrons in Bohr's model of the atom.

Bohr uses the total number of electrons as an ordering principle as can be seen in a lecture published in 1922 but presented in 1913:

"According to Rutherford's calculations the positive charge of the nucleus corresponds to a number of electrons equal to about half the atomic weight. This number coincides approximately with the number of the particular element in the periodic system and it is therefore natural to assume that the number of electrons in the atom is exactly equal to this number. This hypothesis, which was first stated by van den Broek (1912) opens the possibility of obtaining a simple explanation of the periodic system." (Bohr, 1922, p.7-8).

The numbering of the nuclear charge is used to determine the number of the electrons in this "hypothesis". However, no periodicity is mentioned here. Bohr expresses his ideas on periodicity in the informal hand written note to Rutherford, known as "The Rutherford Memorandum" (Bohr, 1912, spelling as in the original handwriting):

"It is however immediety seen that there is an essentially difference between the stability of rings containing a diffrent number of electrons, as it can be shown that the energy of an electron in the ring (the sum of kinetic energy and the potential energy relative to the kern and the other electrons) is negative if $n \leq 7$, but positiv if $n > 7$, and that therefore an electron of a ring containing more than sewen electrons is able to leave the atom. It is therefore a very likely assumption that an atom consisting of a single ring, cannot contain more than sewen electrons. This, together with the fact that inner rings of electron in Prof. Rutherfords atom-model, will have only very little influence (and always to the worse) on the stability of outer rings, seems to offer a very strong indication of a possible explanation of the periodic law of the chemical properties of the elements (the chemical properties is assumed to depend on the stability of the outermost ring, the "valency electrons") by help of the atom-model in question." (Bohr, 1912, p.A1)

I point to the evidence that Bohr, in this early stage, was thinking of periodicity with a stable ring of seven or fewer electrons. Some time later, he based his assumptions of a single ring of seven electrons on spectral data, i.e. a physics context (Bohr, 1913b, p.482). However, in the case of the structure of atoms containing a larger number of electrons, he presumes that the number of electrons in the inner rings "will only be 2, 4, 8 ...", meanwhile referring to chemical properties:

"This assumption in regard to the number of electrons in the rings is strongly supported by the fact that the chemical properties of the elements of low atomic weight vary with a period of 8." (Bohr, 1913b, p.495)

Chemical properties are also mentioned when the number of electrons in more than one ring is proposed:

"The particular member of the series of the elements for which the four innermost electrons will be arranged for the first time in a single ring cannot be determined from the theory. From a consideration of the chemical properties we can hardly expect that it will have taken place before boron ($N=5$) or carbon ($N=6$), on account of the observed trivalency and tetravalency respectively of these elements; on the other hand, the periodic system of the elements strongly suggests that already in neon ($N=10$) an inner ring of eight electrons will occur." (Bohr, 1913b, p.495)

It is evident from these quotations that Bohr used phenomena from the chemistry context like observed tri- and tetravalency to represent periodicity and to account for the number of eight electrons in the development of his model of the atom and the design of the electron configuration.

The Periodic Table is not based on one specific experimental result from chemistry or physics alone, or on one particular theoretical assumption. Instead, the Periodic Table is established by means of a fruitful combination of phenomena and theoretical notions from both contexts, the periodicity being dependent, in principle, on chemical phenomena.

2.4.2 Formation of methane, change of context or hybridization

The second example of the combination of chemistry and physics contexts is a less successful one.

Bohr was of the opinion that he could describe the *constitution of molecules* with his theories (Bohr, 1913a, p.3). More and more, he had to reconsider this idea because he could not use earlier assumptions and representations e.g. that electrons move in circular orbits. He could describe the formation of a hydrogen molecule and also explain the non-existence of a helium molecule He_2 . In the case of the formation of a methane molecule CH_4 , however, he reports difficulties:

"In the preceding we have only considered systems which possess an axis of symmetry around which the electrons are assumed to rotate in circular orbits. In systems such as the molecule CH_4 we cannot, however, assume the existence of an axis of symmetry, and consequently we must in such cases omit the assumption of exactly circular orbits. The configuration suggested by the theory for a molecule of CH_4 is of the ordinary tetrahedron type; the carbon nucleus surrounded by a very small ring of two electrons being situated in the centre, and a hydrogen nucleus in every corner. The chemical bonds are represented by 4 rings of 2 electrons each rotating around the lines connecting the centre and the corners. The closer discussion of such questions, however, is far out of the range of the present theory." (Bohr, 1913c, p.874)

Later, he abandons the molecular models with "electron rings" as "valence bonds", indicating that the configuration in a tetrahedron is important in explaining the structure of organic compounds. He distinguishes between molecular structures of, for instance,

organic compounds and those "in which the individual atoms occur as electrically charged ions" (Bohr, 1922, p.93). While he claims that his model of the carbon atom originates from a consideration of the stability of the whole atom, he cannot include the spatial symmetry of a tetrahedron in this atom model. He denotes as his main purpose "to consider the fitness which the configurations of the electrons offer in the various atoms for the formation of ions" (op. cit., p.93). This and the use of the terms "hetero-polar" and "homeopolar" point in the same direction as Van Arkel and De Boer in their textbook 'Chemische Binding als Electrostatisch Verschijnsel' (Van Arkel and De Boer, 1930).

In the chemistry context the explanatory power of Bohr's model of the atom is restricted to the formation of ions. Although electrovalency can be explained by this model, it does not provide an explanation of the formation of molecules or covalency.

With regard to the formation of a methane molecule, the chemistry context of that period in history offers a more adequate explanation, presented by Lewis.

Bohr and Lewis published their ideas at almost the same time and in a comparable manner. The book 'Valence and the Structure of Atoms and Molecules' by Lewis (1923) appeared a year later than the collection of three essays by Bohr (1922). Also, Lewis' article (1916) was published later than Bohr's trilogy (1913). On the other hand, Lewis' first drawings of the cubical atom were made in 1902 while the first version of Bohr's model of the atom dates from 1912.

Bohr referred to the Periodic Table in the case of the number of eight electrons. It seems that Lewis also looked there for the number of eight (Lewis, 1923, p. 27). However, in the 1916 article, he decided on this number in a different way. His third postulate was:

"The atom tends to hold an even number of electrons in the shell, and especially to hold eight electrons which are normally arranged symmetrically at the eight corners of a cube." (Lewis, 1916, p.768)

Working out this postulate, Lewis processed formulae representing the composition of substances in such a way that the number of electrons in the "atomic shells" was recorded. These numbers of electrons in the outer shells are quite often a multiple of eight, and in almost all cases, an even number. For instance, H_2O : $2 \times 1 + 1 \times 6 = 8$; K_2CO_3 : $2 \times 1 + 4 + 3 \times 6 = 24$. Of the thousands of compounds considered, only a few are known to have an odd number of electrons, for instance NO. Lewis expressed his interest in these compounds because of their reactivity. He called molecules of these substances odd molecules "which contain an odd or unpaired electron" (Lewis, 1916, p.771).

Lewis' comments on Bohr's theories were rather critical:

"Indeed it seems hardly likely that much progress can be made in the solution of the difficult problems relating to chemical combination by assigning in advance definite laws of force between the positive and negative constituents of an atom,

and then on the basis of these laws building up mechanical models of the atom. We must first of all, from a study of chemical phenomena, learn the structure and the arrangements of the atoms, and if we find it necessary to alter the law of force acting between charged particles at small distances, even to the extent of changing the sign of that force, it will not be the first time in the history of science that an increase in the range of observational material has required a modification of generalizations based upon a smaller field of observation. Indeed in the present case, entirely aside from any chemical reasons, a study of the mathematical theory of the electron leads, I believe, irresistably to the conclusion that Coulomb's law of inverse squares must fail at small distances." (Lewis, 1916, p.773)

I see in this quotation an argument for "*starting from phenomena*" in the chemistry context, such as chemical combination and composition of substances. The applicability of a law from the physics context, viz. Coulomb's law at small distances, is questioned.

The first design of Lewis' cubical atom had its drawbacks. It could be used to explain the formation of ionic compounds and non-polar substances and it could also represent the formation of single and double covalent bonds. However, it was not suitable for representing the carbon atom bonded to four other atoms. For this reason, Lewis regrouped the eight electrons on the corners of the cube to electron pairs on the corners of a tetradron. This tetradron model had other advantages over the earlier proposed form because:

"With the cubical structure it is not only impossible to represent the triple bond, but also to explain the phenomenon of the free mobility about the single bond which must always be assumed in stereochemistry." (Lewis, 1916, p. 780)

Lewis decided to adjust his model because of chemical knowledge about the existence, composition and structure of substances.

In my interpretation, this is an example of a combination of theory and phenomena that is successful, however, only within the chemistry context.

An example of a combination of the chemistry and the physics contexts that is successful but also regarded as controversial, is the case of hybridization. The name of Pauling is connected with this concept. He considered hybridization necessary because of stereochemical data. How can a free carbon atom with 2s and 2p orbitals account for the formation of four identical chemical bonds? The following description dates from the period when quantum theory could be regarded as 'under construction':

"There are four orbitals in the valence shell of the carbon atom. We have described these as the 2s and the three 2p orbitals, with bond strengths 1 and 1.732, respectively. These are, however, not the orbitals used directly in bond formation by the atom. (They are especially suited to the description of the free carbon atom; if quantum theory had been developed by the chemist rather than the spectroscopist it is probable that the tetrahedral orbitals described below would

play the fundamental rôle in the theory, in place of the *s* and *p* orbitals.)" (Pauling, 1939, p.81-82)

This combination of aspects from the chemistry and physics contexts has resulted in an application of quantum theoretical notions in organic chemistry. However, how this attempt is rated depends on the context from which it is viewed. And this is related to the meaning of hybridization, which also depends on the context. Hybridization in a structural formula of methane is depicted by equivalent positions of the H atoms in relation to the central C atom, representing the equivalency of the four hydrogen mass portions in a reaction, for instance substitution by halogen. Hybridization can also be regarded as a mathematical operation in a quantum theoretical sense.

Compared to the productive combination of chemistry and physics contexts in the case of the Periodic Table, the formation of a methane molecule from one carbon atom and four hydrogen atoms may be regarded as a problematic combination of these contexts. Data from the physics context, such as spectra, are sometimes less suitable to describe bonds or the formation of bonds such as in CH₄. *In the case of chemical theories related to the formation and structure of molecules, phenomena from the chemistry context are prevalent. Moreover the decisive role of phenomena in developing and evaluating theories is such that phenomena should be considered as the starting point when discussing theories or describing the formation of theories.*

Therefore, strong reductionism is here too to be rejected with regard to the reduction of phenomena to theories.

In this part of the educational analysis of chemical bonding I extend the description of the gap as a gap between the chemistry context and the physics context, not only in textbooks for secondary and university education, but also in the history of science itself. The educational sequence of topics (a physical introduction to chemical bonding) appears to be related to a reductionistic conception of science and scientific theories. Reduction of theories is not generally accepted among scientists. Rejecting the conception of strong reduction implies accepting that chemical theories cannot be derived from physical theories. Scientists who adopt this view, favour a pluralistic conception of science. This could mean that, in their view, the contexts exist side by side and independently, and that profitable relations are possible in either direction. An example of a fruitful combination of phenomena and theoretical notions from both contexts is the Periodic Table. The description of the formation of a methane molecule is an example in which chemical phenomena are prevalent. The importance of phenomena for the formation of theories is another reason to regard reductionism in science with caution.

The following questions are posed in Chapter 1:

- Can chemical bonding be explained by starting from the structure of the electron cloud as described in Hoofdstuk 10?

- What explanations of chemical bonding are accepted by contemporary chemists and what is the role of physical theories in such explanations?

The answer to the first question is that this explanation is not successful; only the formation of positive ions can be accounted for.

With regard to the second question, contemporary scientists do not agree about which explanations of chemical bonding are preferable. The role of physical theories, and quantum mechanics in particular, is important but no consensus exists as to whether chemical bonding could or should be explained from first principles of this theory. A pluralistic conception of science could well be the prevalent view.

In the next chapter, I intend to go into the consequences of a pluralistic conception of science. Since parts of the theories of Bohr and Lewis deal with drawing up and using models of molecules and atoms, I will consider the model aspects of the descriptions of free and bonded atoms, and working with models. Models and working with models should imply aspects of reductionism, and here, the two-step thesis of reduction is relevant. I will explore this two-step thesis of reduction with respect to models and working with models as part of the educational analysis of chemical bonding.

3 Chemical Bonding and Working with Models

In this chapter I continue the educational analysis of chemical bonding in molecules by looking into models and how they are introduced. In Chapter 1 I mentioned models, when describing the major inconsistency, the 'gap', in terms of two models, *viz.* a model of the free atom and a model of the atom bonded in a molecule. In chemistry, as in all empirical sciences, models are regarded as an integral part of theories, as research tools. Models on chemical bonding are corpuscular in nature. Therefore, working with models in chemistry has a special feature in that a conception of a corpuscular nature of matter must be accepted before the models can be used in theories.

First, in Section 3.1, I look into the reasons why models are relevant for chemistry education. I discuss an interpretation of the thesis of reduction (cf. Section 2.3) with regard to models and I relate the two steps in the thesis of reduction to the *acceptance* and the *use* of corpuscular models. I associate what I call a 'minima naturalia dilemma' in chemistry education with the first step of the thesis. How three different textbooks present corpuscular models as models will be analyzed in Section 3.2. In Section 3.3 I will put forward three methods of introducing the use of corpuscular models, i.e. the second step, in chemistry education. These methods are related to a view on the characteristics of models and their application in scientific practice. By combining methods of introducing models and characteristics of models, a classification table is constructed. This table is used when looking into the introduction of models for chemical bonding (Section 3.4) and molecular shape (Section 3.5) as presented in the three textbooks mentioned above.

To conclude, in Section 3.6, I discuss the results of this chapter in relation to teaching and learning about models and I formulate criteria for designing teaching material.

3.1 Models and the Corpuscular Nature of Matter

3.1.1 Models, formal and canonical

In view of the results of the analysis of Hoofdstuk 10, it is worthwhile to examine what models are and how models can be recognized as models. A reason for introducing models and their uses in chemistry education is their relevance to the *methods of chemistry*, especially when theories are studied.

Gilbert and Boulter argue that, as models are among *the main products of science*, education in science must include a knowledge of the major conceptual models used (Gilbert and Boulter, 1994, p.329).

According to Keller (1977, p.42), *the process of thinking in terms of models*, especially with regard to the relation between structure and property, is very important in science education if students are to gain knowledge and insight.

Introducing models in chemistry education should include a discussion on models as a product or models functioning in a process. An obvious question is whether the role of models is, or can be the same in science and science education.

In this respect I consider two fundamental aspects of models which need to be understood in order to be able to work successfully with models.

(i) It should be stressed that a model is *not the reality of an object or event*, for instance, a white crystal:

"Model in the technical-scientific domain is a depiction of the reality, made by restriction and simulation of the reality with the aim of acquiring knowledge."

(Keller, 1977, p.4)¹

(ii) Furthermore, a model is *not the idea itself*, for instance, molecular shape: "A model is a representation of an object, an event, or an idea" (Gilbert and Boulter, 1994, p.328; cf. Gilbert, 1993, p.5)

According to my interpretation of these two remarks, the model is not the object but a *representation or depiction* of that object, be it real or abstract.

A model is not reality and it is not a conception of reality. This status of models should be kept in mind when building up students' understanding of the model concept as they gain experience with it in chemistry education.

The distinction with regard to models as a product is linked to a distinction often made between a material and an immaterial, formal model. The latter distinction has a bearing on how models are introduced and how students learn to understand and work with them.

Material models, such as scale models, are suitable for systems or objects that can be observed but are too complex, too large or too small to investigate directly. On the other hand, thought constructions or formal models function as models of abstractions or hypothetical objects. These formal models are communicated in the form of texts, symbols, or drawings (De Vos, 1985, p.92). De Vos uses the expression "mental" model, not meaning a personal model but an immaterial, abstract model. In this thesis I think it appropriate to use the term 'formal' instead. However, the use of these formal models can be complicated because there is also the possibility of describing, drawing or making material models of the formal models. An example is the ball-and-stick model of molecular structures.

¹ "Modell im technisch-wissenschaftlichen Bereich ist eine nach Einengung und Simulation der Realität zum Zwecke der Erkenntnisgewinnung erstellte Abbildung der Realität." (Keller, 1977, p.4)

When the process aspect of models in science is considered, other distinctions can also be described.

One distinction is between personal and canonical models: whether a model is developed and upheld by an individual or accepted and shared by a community of participants in the scientific discussion.

Gilbert and Boulter distinguish between a personal, *mental* model and a *conceptual* or *consensus* model. A mental model is formed whenever a person tries to comprehend an idea or solve a problem. A conceptual or consensus model is a model which is available to all scientists and which is generally accepted and socially agreed by them (Gilbert and Boulter, 1994, p.328; 1995, p.1). I relate the consensus model to a canonical model as described by Van Oers.

Van Oers (1988, p.128) calls models that are accepted by the scientific community *canonical* models. In his view, *gathering knowledge in science* is accompanied by *discussion about models*. He argues that the discussion of personal and canonical models is a fundamental condition for scientific progress (Van Oers, 1988, p.130). In his cultural-historical approach to education, discussing personal models should be like an educational imitation of scientific thinking.

The reasons for introducing models and their use in chemistry education are related to the model as a product as well as to the process of working with models.

Students need to know the main models used in chemistry. Obviously, corpuscular models occupy a central position in this field. The ability to work with such models is an important teaching goal. But how will corpuscular models retain the status of model which they have in chemistry as a science, when introduced in chemistry at school?

In my view the process leading from personal models to generally accepted, canonical models is not only a feature of science but should also be a feature of pre-university scientific education. However, imitating scientific discussion or imitating the process of designing scientific models is difficult, because the aim in science is to reach consensus on models leading to the establishment of canonical models. *In education, the corresponding aim is to teach accepted, canonical models and there is no freedom to change them.*

3.1.2 Representing reality

In the preceding chapter I discussed various aspects of the relation between the chemical and physical contexts (Section 2.3). Although I argued against the strong reduction of chemical theories to physical theories, it is not possible to object to reduction as such, because methods in chemistry inevitably include reduction. This is the case every time complex systems are reduced to more 'simple' subsystems or "Teilsysteme". The chemist's aim is often to explain complex systems by describing the properties and the behaviour of its subsystems (cf. Primas, 1985a, p.109. See also Section 2.3).

Chemists investigate the phenomena of matter, or more specifically, substances, and therefore the first step must be to *accept* the idea of subsystems of substances. The second step is to *use* these subsystems in describing and explaining the behaviour of substances in a theoretical framework. *To accept and to use the idea of subsystems of substances is what the two-step thesis of reduction means with regard to corpuscular models.*

In the theoretical context of explaining chemical phenomena, the subsystems of matter to be accepted in chemistry are molecules and atoms. According to Rip:

"Therefore, an explanation that makes use of molecules and atoms always involves two steps: first postulating a specific ontology (what entities exist in this invisible world (i.e. the world behind the phenomena)), and then postulating a theoretical network of relationships between these entities." (Rip, 1996, personal communication)²

In my interpretation of the formulation given above, explanations by means of molecules and atoms is the second part of a two-step procedure which I relate to the two-step thesis of reduction.

The conceptions regarding molecules and atoms reflect a discontinuous conception of matter which assumes that matter is particulate, or corpuscular, in nature. This leads to discussions on how these particles or corpuscles can be represented in models.

I agree with De Vos when he writes on the distinction between the corpuscular hypothesis and corpuscular models:

"From an educational point of view it is important to distinguish between the *hypothesis* that matter has a corpuscular structure on the one hand, and *representations* of this structure on the other hand. This is because the object-model relationship is not between matter as it presents itself to us and the corpuscular representations, but it is between matter *conceived of as corpuscular* and corpuscular representations. First, the hypothesis that matter has a corpuscular structure must be accepted, only then does it make sense, since the corpuscular structure appears to have a low accessibility to research, to design a model as a research tool." (De Vos, 1985, p.94. De Vos' italics)³

Although this was written with regard to the use of models by pupils starting to learn chemistry, more advanced students must also be aware of the hypothetical aspects of the corpuscular nature of matter and of model aspects of molecules and

² "Een verklaring met behulp van molekulen en atomen bestaat dan ook altijd uit twee stappen: het postuleren van een bepaalde ontologie (wat voor entiteiten bestaan er in die onzichtbare wereld (i.e. de wereld achter de verschijnselen)) en het postuleren van een theoretische samenhang tussen die entiteiten." (Rip, referring to his contribution on a survey conducted by Van Berkel in 1993).

³ "Het is vanuit onderwijsgezichtspunt belangrijk onderscheid te maken tussen enerzijds de *hypothese* dat materie een korpusculaire structuur bezit en anderzijds de van deze structuur gemaakte *voorstellingen*. De objekt-model relatie bestaat nl. niet tussen de materie zoals ze zich aan ons voordoet en de korpusculaire voorstellingen, maar tussen de *als korpusculair opgevatte* materie en de korpusculaire voorstellingen. Eerst moet de hypothese dat de materie een korpusculaire structuur bezit worden aanvaard, pas daarna heeft het zin van deze korpusculaire structuur, die moeilijk toegankelijk voor onderzoek blijkt te zijn, als hulpmiddel bij onderzoek een model te ontwerpen." (De Vos, 1985, p.94. De Vos' italics)

atoms. Having accepted this, they are better equipped to answer questions about chemical bonding.

The subsystems, molecules and atoms, are not portions of the systems of substances because the subsystems are supposed to be more 'simple', i.e. in the sense of being less difficult to examine. Therefore it is not possible to describe the molecules and atoms themselves as small portions of the substance (as the name 'particle' suggests), but only to describe *representations* or *models* of these subsystems. *I link the first step of the thesis of reduction, in which the hypothesis of the subsystems is accepted, to the corpuscular hypothesis of De Vos. The second step of the thesis, the use of models, I link to the corpuscular models designed as tools.*

The first step of accepting the subsystems, in this case corpuscles such as molecules and atoms, is not a simple one for various reasons.

A very important problem associated with this step regards the relation of the subsystems to the reality of phenomena and to the hypothetical aspects of the corpuscular nature of matter which are often neglected in 'chemical everyday life'.

Keller (1977) states that:

"On the basis of observation, models are designed from which conclusions are drawn regarding the properties and behaviour of atoms and molecules; this means that all statements by chemists about atoms and molecules have model characteristics". (Keller, 1977, p.15)⁴

I distinguish two implications of this statement when comparing it with the first step of accepting molecules and atoms as subsystems. Both implications are closely connected with the meaning of reduction and with the corpuscles being very small (and very large in number) and more 'simple'.

The first implication has to do with chemical language and the use of that language (De Vos and Verdonk, 1987a, p.692). Chemists describe phenomena in macrochemistry by using *phenomena terms*. (For instance colour, melting point, and a specific crystal shape.) The corpuscular nature of matter and its representation is associated with microchemistry (or submicrochemistry, cf. Johnstone, 1993, p.703). When chemists speak about microchemistry and the models of the subsystems they use *model terms*. (For instance molecule, atom, electron, bond, crystal lattice and energy level.) The language of chemistry, written or spoken, is characterized by a 'toing and froing' between microchemistry and the macroworld of substances and reactions. *Chemists are accustomed to using a mixture of model terms and phenomena terms which can be very confusing for non-chemists or for chemists-to-be when they do not know when or which models are used.* Moreover, the hypothetical aspects of the

⁴ "Über den Beobachtungen werden Modelle aufgebaut, aus denen auf Eigenschaften und Verhalten der Atome und Moleküle geschlossen wird; das bedeutet nicht mehr und nicht weniger, als dass alle Aussagen der Chemiker über den atomaren Bereich Modellcharakter tragen." (Keller, 1977, p.15)

corpuscular nature of matter are seldom mentioned: the first step is often neglected because chemists take that step for granted.

The second implication which I associate with the first step of the 'thesis of reduction' arises in chemistry education when students use subsystems in a non-reduced way, i.e. not 'simple'. In such cases, molecules are seen as having the same properties as the substance itself (cf. Ben-Zvi, Eylon and Silberstein, 1986; De Vos and Verdonk, 1987b). I call this the *minima naturalia dilemma*.

De Vos (1985, p.104) mentioned the *minima naturalia* when he referred to small subsystems and their development in history (cf. Dijksterhuis, 1985).

It was assumed by scientists in the Middle Ages that the subsystems retain all the properties of the substance as a whole. If sulphur molecules are described as yellow or a water molecule as wet, only part of the first step of the reduction is made, *viz.* the divisibility into subsystems, and not the remaining part, the reduction to 'simple' subsystems. Yellow and wet molecules are *minima naturalia* rather than molecules. These minima can be useful for explaining phenomena associated with the smallness and the extremely large number of the subsystems, but not for explaining colour or wetness. On the contrary, in order to explain these phenomena the first step must be completed, and only then can models of the 'simple' subsystems be constructed.

The question is how models and the use of models are introduced in textbooks with a view to teaching pre-university students about the content and the procedures of scientific research. I am interested in the answers to this question because these answers combined with the results of the Hoofdstuk 10 project could help to get a better idea of how to design a teaching sequence on chemical bonding with appropriate models. Analyzing other textbooks helps to gain more insight into developing ideas and gives an opportunity to test tentative ideas.

Sofar I have discussed an interpretation of the two-step thesis of reduction in relation to models in chemistry. The first step is accepting corpuscular models. Before going into the second step, the use of such models (Section 3.3), I will examine how corpuscular models are introduced in three textbooks and thus how the first step of the thesis of reduction is taken.

3.2 Corpuscular Models in Three Textbooks

Three American textbooks were chosen for examining the introduction of corpuscular models. In the following discussion I use the code names: ChemA, ChemM and ChemP⁵. These books are suitable for my purpose because they are all fairly recent,

⁵ ChemA: CHEMISTRY. Wilbraham, Staley, Simpson and Matta (1987, 1990).

ChemM: CHEMISTRY, a Modern Course. Smoot, Smith and Price (1987, 1990).

ChemP: CHEMISTRY. The Study of Matter. Dorin, Demmin and Gabel (1989, 1992).

dating from the same period as CHEMIE 5/6V (1985), they are approximately the same size and are all single-volume texts. All three include the same material but present it more comprehensively than Hoofdstuk 10. The material is arranged in the same order, although in chapters and not in sections: a chapter on 'Atomic Structure', followed by a chapter dealing with the configuration of electrons in an atom, and then a chapter or chapters on chemical bonding. I presume the order of these chapters to be determined by a reductionist conception of science.

To see whether the acceptance of models can be described with the two-step 'thesis of reduction', I will look into the way the hypothesis of corpuscular models is postulated in the three textbooks. Therefore I examine first what is incorporated in the glossary and in the text on the particulate nature of matter and then what the books say about the hypothetical aspects of models.

I examine the sentences with the terms matter, atom and element in the introduction of the particulate nature of matter (terms in italics were found as such in the glossary) to see whether the chosen subsystems are 'more simple' or are 'parts of the whole', and if model terms are used.

ChemA:

"*Matter* is anything that takes up space and has mass." (5 and cf. 696)

"By the late 1800s scientists were convinced that atoms are the fundamental units of which all matter is composed. (67)

This particle is an *atom*, the smallest particle of an element that retains the properties of that element." (67 and cf. 690)

"*Element*: a substance that cannot be changed into a simpler substance under normal laboratory conditions." (693)

ChemM:

"Chemists have found that there is a very close relationship between the structure of matter (how it is put together) and the properties of matter (how it behaves). For instance, a diamond is very hard. It is hard because of the way its atoms are held together." (3)

"According to the atomic theory, matter is made of very tiny particles called atoms." (44)

"*Matter*: anything that exhibits the property of inertia." (672)

"*Atom*: the smallest particle of an element." (666)

"*Element*: a substance whose atoms all have the same number of protons in the nucleus." (669)

ChemP:

"The modern view of matter is that every sample of matter consists of very small particles." (101)

"Today scientists believe that atoms are the fundamental building blocks that make up all matter." (109)

"*Matter*: anything that occupies space and has mass." (804)

"*Atom*: the smallest particle of an element that can enter into chemical change. It consists of a central nucleus and electron clouds outside the nucleus." (799)

"*Element*: a substance that cannot be decomposed into simpler substances by ordinary chemical means." (802)

Discussion

In all three books the discontinuous nature of matter is expressed by 'particulate' or 'particle'. The term 'particle' suggests that it is a part of a whole, a view that easily evokes minima naturalia ideas. By using the expression 'corpuscle', instead of 'particle', a distinction is possible between a theoretical and a phenomenological point of view. In order to express a difference and to stress the reductionistic aspects of the discontinuous nature of matter, I prefer the terms corpuscle and corpuscular to particle and particulate.

- The distinction between phenomena terms and model terms is illustrated by the definition of an atom in the glossary of ChemP: the first sentence can be interpreted as referring to the phenomenon of chemical change, whereas the second sentence belongs to a theoretical model context. Another example is the definition of elements which is stated in phenomena terms in ChemA and ChemP, and in model terms in ChemM.

- There seems to be a difference between statements from a scientist's point of view, and facts presented in the framework of teaching. When expressions such as 'scientists believe' or 'chemists have found' are used, it seems that scientists may doubt or can be convinced. However, students must accept and learn the facts they are reading about in the text.

The quotations indicate that the corpuscular nature of matter is not introduced as something that *might be* accepted but, rather, that facts are given which *are* generally *accepted* by scientists. The canonical aspects of the nature of matter are not a point of discussion.

It seems that the *acceptance* of corpuscularity, i.e. the first step of the 'thesis of reduction', is not included in the design of this teaching material. Of course, it might be dealt with in the practice of teaching.

In examining whether attention is paid to the hypothetical aspects of corpuscular models as models, I look into the statements on models in the three textbooks to see whether they mention assumptions or the kind of model.

ChemA:

"*Theory*: a thoroughly tested model that explains why experiments give certain results." (3 and 700)

"The scientific method incorporates observations, hypotheses, experiments, theories, and laws. ... Hypotheses are descriptive models for observation." (3)

"A theory can never be proved. Nevertheless, theories are very useful because they help us to form mental pictures of objects or processes that cannot be seen."

(3)

ChemM:

"*Model*: an arrangement analogous to, and useful for, understanding a system in nature, but existing only in one's mind." (672)

"The relationship between properties and structure can be organized into several basic principles, facts, and theories. A theory is simply an explanation of some relationships." (5)

"Scientists often develop models in their minds to help deal with abstract ideas and objects. ... Chemists often build mental models. ... plumpudding model of Thomson ... the planetary atom." (9)

ChemP:

"A good model of the atom helps to explain the characteristics and behavior of atoms. But it is not an actual picture of an atom." (125)

"*Scientific model*: A mental picture that helps to explain something that cannot be seen or experienced directly." (807)

"*Scientific method*: The manner in which scientists proceed to solve a problem. They state the problem, collect observations, search for scientific laws, form hypotheses and theories, and modify these theories when necessary." (807)

"Such an educated guess, based on observed facts, is called a *hypothesis*." (3)

"A theory shows a relationship between observations that at first seemed totally unrelated. A theory, therefore, unifies many pieces of information to produce a grand design." (3)

"*Theory*: (1) An explanation of observed relationships that has been verified to some extent. (2) An intellectual scheme that unifies a great many observed facts, such as the cell theory, atomic theory, theory of continental drift." (808)

Discussion

In these quotations, it can be seen that some of the various definitions or descriptions of the term 'model' are related to a theoretical context. I conclude this from the relationship with accompanying terms, such as, 'theory', 'hypothesis', and 'scientific method'. On the other hand, observations are also mentioned. Apparently, the model has an intermediate function between observation and theory.

- In the theoretical context of ChemA, the concept of a model would seem to be that of a formal model. However, the use of the word 'pictures' could give the idea that it is a drawing of the objects or processes as they really are, if only they could be seen. It is not clear whether 'mental' is used in the sense of personal or in the sense of formal and conceptual. The examples, plumpudding model and planetary model, given in ChemM seem to imply that a conceptual model is meant, and moreover, that a model of a model is given.

- In each of the three textbooks a different view on models is found. In ChemA, a model is seen as a prototheory, whereas the link between model and theory in the other books is not made clear. A model "helps to explain" in ChemP, but the meaning of "deal with" in the ChemM description of models in scientists' mind is not made clear.

From the statements on models, it can be concluded that the hypothetical aspects of models are taken into account in the three textbooks. It is, however, questionable whether, when the canonical models of chemistry are introduced, they will retain their status as model or be described as reality. As this is part of the second step of the thesis of reduction, the use of models, it will be further discussed in the next sections.

3.3 Characteristics and Introductions of Models Combined

In order to recognize and describe the use of models in the main text of the three textbooks, I need criteria to identify differences and similarities between the models and the way they are used. First I look for characteristics of the use of models in scientific practice (3.3.1) and I discuss three possible methods of introducing the use of models in science education (3.3.2). Then I combine the characteristics and the methods of introduction in a table (3.3.3).

3.3.1 *Characteristics of models in practice*

In the following, I elaborate on a number of characteristics of models in science, identified by De Vos (1985, p.88-92).

The choice of a model depends on the intentions of the researcher and the question the researcher is aiming to answer about the object. Working with models is a research technique designed to answer a research question.

a. A model is a *tool* in a research effort directed at a research object. It is used if the object itself is difficult to examine. The model is used as a temporary, substitute research object.

b. Examination of the model may lead to conclusions that are reformulated as *hypotheses* with respect to the original research object. This allows the researcher to approach the object more directly. The researcher knows what to look for and where to look for it.

c. The hypotheses generated by the model are relevant to the original research object only if there is a certain *correspondence* between the object and its model. In a scale model, such as a map, the correspondence is defined by the scale of the model. In a mathematical model of a chemical system, e.g. an equilibrium, it is given by the meaning of the various symbols used in a formula. The correspondence enables the researcher to formulate the hypothesis in terms of the original research object.

d. The correspondence between object and model would be complete if the two were identical. In that case everything that is known about the model will automatically apply to the object. However, the model will then fail as a research tool since it is just as inaccessible for research as the object itself. A model must therefore

differ from the research object. A model has to be more *simple* than the original object of research, simple in the sense of being less difficult to examine.

e. It is obvious that correspondence and simplification may be conflicting demands. For instance, the simpler the model is, the less it will correspond with the original object. The researcher has to find a compromise. Designing or selecting a model has personal and situational dimensions: a specific model may be highly favoured by one researcher in a specific situation and rejected as too complicated or too simple by a colleague or in a different situation. The design and/or the choice of a model is *subject dependent*. As a model usually contains elements not only from the research object but also from other sources which are supposed to be analogous to the object, at least to some extent, designing a suitable model requires *creativity* on the part of the designer of the model.

f. A model can be of value once again after it has produced several useful hypotheses. If testing the hypotheses leads to new information about the actual research object, it may be possible to adapt or refine the model and use it as a source of new or more accurate hypotheses. This may result again in new knowledge about the research object, and so on. A model figures then as a development tool in an *iterative* research process.

These characteristics of model use should be taken into account when introducing models in education. To what extent this is possible will be discussed in the following subsections.

3.3.2 *Introducing the use of models in chemistry education*

When analyzing Hoofdstuk 10, we got the impression that some of the difficulties with models are associated with the *way* models are introduced and with the model aspects being too implicit.

I will identify and describe three possible methods of introducing the use of models. Each of the approaches allows for a consistent introduction, although not all model characteristics described above are covered by each introduction, as I will show in 3.3.3.

In the first approach, only one *single* model is presented which is designed to explain as many phenomena as possible. Consequently, this model is often a complex one, and might be regarded as fundamental in the theoretical context. An example is a quantum theoretical model seen as preparation for the university. To avoid difficult parts of scientific practice within this one model, such as complicated experiments and mathematical formulas, all kinds of aids can be used, for instance computer simulations of diffraction experiments, or analogies with strings.

The second approach is to present various models in a progression from simple to complex which is often historically determined. Each time a new model is introduced, the previous model is discarded. Each model is therefore regarded as *provisional*, either in the context of the history of science (authentic or as a

construction) or in the context of a sequence based on educational assumptions from simple to complex.

A third approach to introducing models is to present two or more models, use them *simultaneously* and emphasize the *relativeness* of each model. In this approach, various models are in use at the same time, sometimes conflicting, sometimes compatible. When new data become available one must decide whether a new model is needed or whether a model already in use could be used as it is or in an adapted or revised form.

The three ways of introducing models in education are summarized in the following table:

SINGLE	SUCCESSIVE	SIMULTANEOUS
one model, to explain as much as possible definitive model central role of construction	provisional models, from simple to complex rejection of previous models search for next model	relativeness, various models side by side conflicting or compatible adaptation or new design

An example of a one-model approach is the introduction of a quantum model for the atom proposed by Niedderer (Niedderer, Bethge and Cassens, 1990, p.67-80). When teaching only one model, there is a particularly high risk that the model may become a teaching goal in itself, and that what is meant to be an aid or an analogy usurps the central role.

An introduction using provisional models is described in the development of an atomic model in a historical approach by Ben-Zvi (Ben-Zvi, Silberstein and Mamlok, 1990, p.189). A comparable development can be found in CHEMIE 3V/H (1983). Students, however, may feel uncertain about the usefulness of a succession of models and they may ask for the final, 'correct' model. Moreover, they can become confused when a model is still used after having been rejected, as, for instance, is the case with the hard sphere model of the atom.

Examples of a simultaneous model approach with an introduction to the advantages and limitations of various models can be found in Chemistry, a Search to Understand, (Harrison and Weaver, 1989). If a model is rejected, it may still remain useful, albeit within its own, possibly restricted, context. Preference for one model or another depends on the question that is to be answered with that particular model.

In Hoofdstuk 10 of the second edition of CHEMIE 5/6V (1985) the description of the free and bonded atom does not fit into the category of the single model approach, although it seemed to be intended as one model. It is implicit in the text that the description of the structure of the free atom should incorporate all the information

necessary for describing the formation of a bond between two atoms but our analysis has revealed inconsistencies.

An attempt to put the idea of a simultaneous approach into practice is presented in our proposal for the third edition of CHEMIE (CHEMIE 6V, 1993). There a clear distinction is made between the introduction of the model of the free atom with energy levels and that of the molecule consisting of bonded atoms with bonds oriented in space. Later in the text, an assignment is included to compare the two models and discuss their usefulness. Results from a classroom talk are mentioned in Section 1.5.

3.3.3 *Model characteristics and methods of introducing a model*

By combining the characteristics of models (3.3.1) and ways of introducing models (3.3.2), I construct a classification table for comparing the introduction and use of corpuscular models in the three above-mentioned textbooks, ChemA, ChemM and ChemP, in the framework of the second step of the thesis of reduction.

I discuss how and to what extent the characteristics of models can be recognized in each of the methods of introduction.

ad a. In order to see how a model is introduced and used as a tool, there must be some reference to the object of the research. This holds for all three methods: the single model approach as well as the successive and the simultaneous model approaches. However, the number of times the research object is referred to may not be the same with all approaches. With a single model approach, the model as a tool must be mentioned at least once during the introduction, either in the designing phase or during the justification of the choice of the model. In the successive model approach the tool characteristic must be mentioned at least whenever a model is to be replaced by a new one. This also accounts for the simultaneous model approach, although at different moments when using them.

ad b. With regard to the hypotheses developed by using models, there is an opportunity to mention the hypotheses explicitly only at the end with the single model approach while this can be done at various points with the other two approaches.

ad c. The correspondence criterion requires a *matching context* for the model and the object. For example, if the energy aspects of the object are under investigation, the model must have energy features corresponding to energy aspects of the object. The single model approach requires the same context throughout; in the other approaches the context depends on the model-object relation under consideration.

ad d. If the model has to be 'rich' in the sense of producing a variety of potential hypotheses, a single model is likely to be complex, although it has to remain less complex than the object itself. When teaching successive models in the historical order, it is often assumed that there is a sequence from a 'simple' model to complex models. In the simultaneous model approach there is the possibility of a complex model occurring next to a 'simple' one.

ad e. Considering the role of the creative subject, attention should be drawn to how active 'we' or 'you' can be. The introduction leading to canonical models makes it impossible to adapt or change the model or the models to be taught. One can only discuss decisions made by others and the why and wherefore of the model design. In this framework, it is possible to *comment* upon the decisions taken and the usefulness of the models. This can be regarded as part of the *process* of the use of models.

ad f. The last criterion is related to the previous one and concerns the scope for critical reasoning in the iterative process of selecting and developing models. Comparing different models and commenting on the applicability can be done when a number of models is used simultaneously; discussion of whether or not to discard a model turns up with the successive model approach. With a single model an iterative process is not possible.

As the points mentioned under e. and f. are related to each other in describing the scope for discussing and commenting on the use of (canonical) models, these points are taken together as one category in the table.

The following table gives model characteristics and the methods of introducing models in chemistry education:

	a <i>tool</i>	b <i>hypothesis</i>	c <i>correspondence</i>	d <i>simpler</i>	e + f <i>discussions</i>
<i>single</i>	once	at the end	the same	complex	only comment
<i>successive</i>	fixed	several	various	in sequence	yes or no
<i>simultaneous</i>	variable	several	various	mixture	comparing

I will use this table to determine how the use of models, i.e. the second step of the thesis of reduction is introduced in the three textbooks and whether these introductions can be categorized as a single, successive or simultaneous model approach.

Two topics are chosen for consideration, *viz.* chemical bonding (Section 3.4) and molecular shape (Section 3.5), since the gap observed in Hoofdstuk 10 and discussed in Chapter 1 and 2 is seen in relation to chemical bonding and molecular shape.

3.4 Chemical Bonding and the Use of Models

In this section I look into chemical bonding with regard to the introduction and use of models in the three American textbooks. I formulate two questions as a tool for determining differences and similarities. The questions derive from the discussions about the gap:

- Is the occurrence of a chemical bond between atoms a logical consequence of the descriptions of free atoms given earlier in the textbook under investigation?
- Does the description of the free atom belong to the same context as the description of the bonded atom?

First I give a number of quotations from ChemA on chemical bonding, and subsequently I discuss the points that are relevant for the purpose of model introduction and classification.

In ChemA the chapters on bonds are preceded by chapters on the electronic structure of atoms and the organization of the periodic table. Various atomic models are presented in a successive approach up to a quantum mechanical model. Then the electron configurations are introduced as the ways in which electrons are arranged around the nuclei of atoms, followed by the rules of filling the atomic orbitals within the principal energy levels (ChemA, p.251). One of the rules is that electrons enter lower energy orbitals first. In the case of the noble gases, i.e. elements in which the outermost *s* and *p* sublevels are filled, the chemical reactivity, or rather the lack of it, is also mentioned.

The following quotations are from the introduction and the first two sections of the chapter on chemical bonds in ChemA:

ChemA:

"This knowledge of atomic structure and periodicity will help you to understand the chemical bonding that occurs between atoms." (299)

"Knowing electron configurations is important because the number of valence electrons largely determines the chemical properties of an element. Valence electrons are the electrons in the highest occupied energy level of an element's atoms." (299)

"Valence electrons are usually the only electrons used in the formation of chemical bonds. Thus it is customary to show only the valence electrons in electron dot structures. Electron dot structures depict valence electrons as dots. The inner electrons and the atomic nuclei are represented by the symbol for the element being considered." (300)

"Why are some elements found mainly as ions? It is because the nature of things is to adjust to achieve the lowest possible energy. Noble gas atoms are stable. They are of low energy and low chemical reactivity because they have stable electron configurations. (...) In forming compounds, atoms make adjustments to achieve the lowest possible energy. (...) He (*i.e.* Lewis) proposed the octet rule: Atoms react by changing the number of their electrons so as to acquire the stable electron structure of a noble gas." (300)

Discussion

Although it is stated in the first sentence that knowledge acquired earlier will help to understand bonding, the introduction of a cluster of new concepts follows: valence electrons, electron dot structures, octet rule, and stability of the electron configuration of noble gases. Models are not mentioned.

It seems that the conditions for bonding are a specific electron configuration and more specific requirements for stability. In order to be able to form chemical bonds, the atom has to have valence electron(s) on the outer side whereas the inner electrons and the atomic nucleus, both represented by the symbol, are of secondary importance.

Reference is made to the chemical properties of noble gas atoms in order to state the stability of their electron configuration and this configuration is linked also to a specific number by the octet rule.

As some of the above mentioned concepts result from or are associated with the ideas of Lewis, I refer to this 'atom to be bonded' as the Lewis atom, to distinguish it from the free atom in the physics context. A Lewis atom consists of a kernel (the nucleus and the inner electrons) and a possible maximum of eight outer electrons. Eight electrons is the stable number (octet rule). The kernel is often represented by the symbol of the element.

I now compare the statements in the quotations with the categories in the table.

At the beginning of the chapter on bonds, it is implicit that chemical bonding is the topic under investigation. The tool aspect of a model (a) and the hypotheses (b) on chemical bonding are not dealt with. It is only stated that the electron configurations are important in this respect. I conclude that the electron configuration used in bonding requires a distinction between valence electrons and other electrons.

The answer to the question of whether the description of the free atom is from the same context as the description of the bonded atom appears to be negative; the free atom and the bonded atom do not have the same correspondence criterion (c). In the free atom with the (minimum) energy levels the energy context is predominant, while in the bonded atom it is the *position* of the outer electrons, i.e. a distance context, which is important. Although the word 'model' is not mentioned, in my view, two different models are used. By introducing new concepts without explicitly changing to another description or model, the model or description becomes confusing and far from simple (d).

The next characteristic from the table, discussions (e + f), does not apply because there is no opening provided for active participation by the students in choosing or discussing the choice in the introduction.

I conclude that no introduction or discussion of models takes place but that, implicitly, models are used. Not mentioning the model characteristics of the descriptions of chemical bonding might suggest to a reader that a factual description of *real* chemical bonding is given rather than a model.

Using the description of the Lewis atom, which evolved from my examination of the ChemA textbook, I look at chemical bonding in the two other textbooks. In both textbooks model aspects of the atomic models are mentioned in the chapter on the structure of the atom (ChemP) and in the chapter on the electron cloud and probability (ChemM) but no model aspects of descriptions of chemical bonding are mentioned. However, the description of chemical bonding requires new concepts in both textbooks and I examine whether these concepts indicate the presence of the Lewis atom and have the same context for the Lewis atom and the free atom.

ChemP starts by listing the objectives of the chapter on chemical bonding. The first objective is to describe "the nature of the chemical bond and its relation to valence electrons" (p. 389). Then the first section of the chapter continues as follows:

ChemP:

"Today we believe that atoms of different elements combine to form compounds in two general ways (*i.e. by means of ionic bonds and covalent bonds, vHB*). In both ways, the position of one or more electrons in the valence shell of each combining atom is altered. When such a shift in the location of electrons occurs, a force of attraction develops between the atoms involved. This force of attraction, called a chemical bond, holds the two atoms together. The process by which chemical bonds form is called chemical bonding, or just bonding. The formation and breaking of chemical bonds occur during chemical reactions." (389)

"Except for helium, the electron configuration of the valence shell of all the noble gases is s^2p^6 . This arrangement is referred to as the stable octet of electrons. The tendency of valence electrons to rearrange themselves during chemical reactions so that each atom has a stable octet is called the octet rule or the rule of 8." (391)

Chemical bonding is presented here as the rearrangement of valence electrons of different atoms to form a stable octet. In the earlier chapter of ChemP on electron configurations of all the elements, valence electrons have already been referred to as the electrons in the valence shell, or the outermost principal energy level. The condition of having eight electrons in the valence shell is related to the electron configuration of the chemically unreactive noble gases. The arrangement of the valence electrons and the remainder of the atom is described in more detail: the nucleus together with all inner energy levels is called the kernel (ChemP, p.352). However, this description is preceded by that of the electron configuration with the nucleus and the electrons in an orbital diagram and the application of filling rules, whereby the first electron is found at the lowest energy level. In the chapter on chemical bonding, the unreactivity of the noble gases is related to the stability of their electron configuration, and this configuration is later called the stable octet of electrons. Although the Lewis atom is introduced prior to the chapter of chemical bonding, my conclusion is that the description of the Lewis atom as the model of the bonded atom also seems to apply in this textbook.

In ChemM, there is no mention of valence electrons at all, nor are valency or related terms mentioned, but the concept of the electron configuration is used throughout. A new concept, *i.e.* electronegativity, is required for the description of chemical bonding.

ChemM:

"Now that we have examined the structure and properties of atoms in some detail, we are prepared to study how atoms bond to each other to form compounds. The bonds formed between atoms depend on the electron

configurations of those atoms and, also, the attraction the atoms have for electrons." (229)

(...) "Chemists need a comparative scale relating the abilities of elements to attract electrons when their atoms are combined. The relative tendency of an atom to attract electrons to itself when it is bonded to another atom is called electronegativity. The elements are assigned electronegativities on the basis of many experimental tests." (229)

(...) "Electrons are transferred between atoms when the difference in electronegativity between the atoms is quite high." (231)

Remarkably, the tendency of an atom to attract electrons to itself is a property of the bonded atom (ChemM, p.229), but when it is stated that the electrons are transferred, it seems to be a property already existing beforehand in the free atoms (ChemM, p. 231).

In the paragraphs that follow the introduction, the various bond types are discussed, with, for instance in the case of the ionic bond, the stable octet configuration as something to be attained (ChemM, p.233).

Looking for the Lewis atom in ChemM is looking for how the octet rule and how outer electrons and a kernel are introduced.

In the chapter on the Periodic Table:

ChemM:

"When an *s* electron is the highest energy level electron in an atom, it is in the outer level. The same is true of a *p* electron. However, *d* and *f* electrons, theoretically, can never be in the outer level of a neutral atom. Since *s* sublevels hold two electrons and *p* sublevels hold six, the largest number of electrons normally in the outer level is eight. These eight outer electrons are called an octet. We will consider an atom with eight electrons in the outer level to have a full outer level. One of the basic rules in chemistry is that an atom with eight electrons in its outer level is chemically stable, or unreactive. This rule is called the octet rule." (175)

Earlier paragraphs deal with the distribution of electrons among the energy levels according to the arrangements with the lowest energy (ChemM, p.154). On p. 158 the Lewis electron dot diagram is introduced because of the primary concern with the electrons in the outer energy level and their involvement in chemical reactions. The first step in the procedure of drawing dot diagrams is representing the nucleus and all electrons except those in the outer level by the symbol of the element, i.e. the kernel without naming it as such.

Discussion

It can be concluded that in both textbooks, ChemP and ChemM, the free atom is introduced first, followed by the Lewis atom. The change from the context of energy levels to the context of electrons in a special position seems to show similarities with the gap we found when analyzing Hoofdstuk 10. (The same applies to ChemA.)

According to the table (3.3.3), the topic of chemical bonding should be mentioned and hypotheses should be proposed, confirmed or rejected. This has not been done in the three textbooks. It is pointed out that chemists need extra rules to describe bonding more fully, but there is no role for the students. As there is no discussion of why a change of model has taken place or why an extension of the model is needed, it seems that the model character of the atom descriptions is not taken into account. *The conclusion is that what may have been intended as a description of a model, has become part of the description of the object, i.e. chemical bonding.*

The usefulness of the classification table with regard to the categorisation of ways of introducing the use of models could not be tested in this section, because the model characteristics of models of chemical bonding are mostly absent.

However, in two textbooks several models are introduced with respect to molecular shape. Therefore I continue my investigations of how models are introduced and used referring to molecular shape. The main question is now how the gap between the model of the free atom and the Lewis atom is bridged in the case of the carbon atom in a methane molecule.

3.5 Molecular Shape and the Use of Models

In the approach leading from the free atom to the bonded atom, the question in this section is how the gap is bridged with regard to the four equivalent and directed bonds of the carbon atom in the methane molecule. The three textbooks each use a different sequence of the concepts 'shape', 'hybridization' or 'hybrid orbitals', and 'electron pair repulsion'.

ChemP uses overlapping valence orbitals to describe H₂, but then has to introduce hybridization (p. 400) in order to explain with 'promoted' electrons the four identical covalent bonds of carbon in methane. Although the ball-and-stick model of methane is shown in a figure, the tetrahedral shape is mentioned only later in the section discussing the valence-shell-electron-pair-repulsion (VSEPR) model (ChemP, p.406). The VSEPR model is introduced to provide a way to predict shapes of molecules by drawing a dot diagram for the central atom of the molecule under consideration. According to the rules of the VSEPR model, a tetrahedral shape results for the methane molecule with the nucleus of the carbon atom in the center of the tetrahedron. Without comment it is stated that:

ChemP:

"In carbon, it is the four sp^3 hybrid orbitals that account for this structure." (407)

The other two textbooks, ChemA and ChemM, use two different approaches to the directed bonds in molecules and molecular geometry and discuss the merits of having several models or theories.

In ChemM, it is stated in the "Goals" that on completion of the chapter, the students will understand two models used to explain molecular structure (ChemM, p.247). The first sequence of concepts of a model of the structure of molecules to account for their shape is to consider electron repulsion of 'charge clouds', resulting for the methane molecule in "a perfect tetrahedron" (ChemM, p.249). The other model of molecular shape is introduced in the following section with the thought experiment of merging the one s and the three p orbitals to form four equivalent hybrid orbitals, arranged in a tetrahedral shape (p.252).

ChemM:

"Another model of molecular shape considers different ways s and p orbitals can overlap when electrons are shared." (252)

"Instead, according to the model we are considering, the one s and three p orbitals are thought of as merging to form four equivalent hybrid orbitals." (252)

"Because one s and three p orbitals have merged, the hybrid orbitals are represented as sp^3 hybrids. These four orbitals are degenerate and contain one electron each. They are arranged in a regular tetrahedral shape. Each of these hybrid orbitals can then bond to another atom." (252)

"Chemists use different theories to explain molecular structures. Two of these theories are: 1. electron-pair repulsion, (and) 2. hybrid orbital theory." (263, margin text)

"In studying atomic structure we treated the electron as particle, wave, and negative cloud. In studying bonding we have also studied several different approaches to explain what we observe. It is plain that chemists do not have a complete understanding of all factors in bonding. Therefore, more than one explanation is often needed to account for observations.

When faced with multiple explanations, scientists follow a basic rule. That rule is to try the simplest explanation first. If that method does not suffice, then the more complex ideas are applied until one is found to fit. The models of molecular structure presented in this chapter are arranged in order of increasing complexity. Electron-pair repulsion is the simplest model and should be applied first when explaining the structure of a molecule." (263-264)

The sequence of concepts in ChemA is related to the mentioning of several descriptions of covalent bonding, leading to a quantum mechanical description of bonding, without referring to shape, except at the end when p bonding is discussed (ChemA, p.330). In a short interlude attention is drawn to the relation between the properties of a substance and the shape of its molecules as an introduction to the section on the VSEPR theory, and the regular tetrahedron of the methane molecule. The next section is about hybrid orbitals starting with:

ChemA:

"Electron dot structures and the combination of unpaired electrons in boxes representing orbitals are two ways of describing covalent bonding. The VSEPR theory does a good job of describing molecular shapes. Another way to describe molecules that is informative of both bonding and shape is orbital hybridization.

With hybridization several atomic orbitals mix to form the same number of equivalent hybrid orbitals." (333)

In the chapter review of ChemA on molecular shapes (p.344), the VSEPR and molecular orbital models, here called theories, are discussed. The possibility of using either the overlap of atomic orbitals or hybridized atomic orbitals is also discussed, the criterion being which fits the experimental results best. The input of the students in deciding which model or theory to use or which model is preferable can be seen, to a certain extent, in a "challenging problem" on the merits of the different theories (p.347).

Chem A:

"The electron structure and geometry of the methane molecule, CH₄, can be described by a variety of models. These include the electron dot structure, simple overlap of atomic orbitals, and orbital hybridization of carbon." (347)

Students are asked in this assignment what geometry to predict for CH₄ and which picture is preferable, based on the facts of bond angles and bond distances.

Discussion

Hybridization is associated with the carbon atom in the methane molecule. There are two reasons for the gap to exist between the free atom model and the bonded atom model: (i) the four bonds are equivalent and (ii) they are directed in space. *Neither the s and p energy level model nor the atomic orbital model are appropriate for the model of the methane carbon atom.* Using electron pair repulsion, it is possible to account for the tetrahedral shape with the advantage of referring to experimental data on bond angles. The following introduction of a molecular orbital model can be seen as the introduction of another model or theory, however with shape already being something which had been accounted for.

The classification in the table according to molecular shape is a successive approach in ChemM and close to the simultaneous approach in ChemA. In ChemA, several models are compared and related to experimental results. However, the introduction moves from simple to complex as in the successive introduction. The sequence seems to be determined by the 'preference' of chemists for the simplest model or theory.

3.6 Discussing Models and Contexts

In this section I look into the various questions brought forward in this chapter and I link these to questions from preceding chapters. The main question on models in this thesis is formulated in Chapter 1: How can students acquire insight into models and working with models.

I use results of the analysis of three textbooks, either to answer questions or to elaborate on aspects of the questions.

3.6.1 Views on model characteristics

I tried to test the classification table for models using two questions which are dealt with in Section 3.4. Although the questions were meant to be instruments for applying the table in practice, an additional result of testing the table is that I can try to answer these questions. The first question was whether the occurrence of chemical bonds between atoms could be deduced from the earlier descriptions of free atoms in the textbooks.

The word model is not mentioned in the description of chemical bonding in the texts but as I have argued, the interpretation of the texts leads to the identification of two models, one of the free atom and one of the bonded atom. *The two models are different to such an extent that the answer to the question must be negative.*

The answer to the first question is linked to the answer to the second question which is on the contexts of the descriptions of free and bonded atoms. I argued that the descriptions of the free atom and the bonded atom differ in several respects. In my interpretation of the texts, I identify two different models that are presented and used for two different purposes: the free atom model for explaining spectra and the Lewis atom for explaining chemical bonding. These models could not be classified in the table with regard to being a tool and to generating hypotheses. However, in that framework, the requirement of correspondence between 'that to be explained' and its model is still valid. *The correspondence characteristic requires the energy context for the free atom with the energy levels, and the distance/spatial context for the bonded Lewis atom with the position of the valence electrons on the outside of an atom.*

In the following table some of the features of the two models are summarized:

FREE ATOM	LEWIS ATOM
- nucleus and electrons	- kernel and valence electrons
- notation: $1s^2 2s^2 2p^1$ [Ne] $3s^2 3p^1$ [↑↓] [↑↓] [↑] [↑]	- notation: · $\overset{\cdot}{\underset{\cdot}{\text{Al}}}$ ·
- atom, free	- atom, free or bonded
- stability required by minimal potential energy	- stability required by noble gas configuration
- all numbers of electrons possible <106, minimal energy	- numbers of electrons limited determined by octet rule
- configuration of electrons determined by Aufbau with Pauli principle	- position of (valence) electrons determined by repulsion and Pauli principle
- irregularities with 4s - 3d	- irregularities with rule of 2 and 10

Although models are not mentioned as such, they can be traced by using the correspondence characteristic and context. The transition from one model to another can be seen as going from a energy context to a distance/spatial context. The energy context is recognized by the attribution of the electrons to energy levels and the requirement of minimal energy. The distance/spatial context is defined by the requirement that the valence electrons have positions on the outside of the atom. Since the models correspond to two different contexts, the transition from one model to another can be seen by comparing contexts.

The classification table was designed to classify the ways in which the use of models is introduced in chemistry education. As I have argued, classification is not possible in the case of chemical bonding, because model characteristics are not dealt with in the introduction. The case of molecular shape showed that by engaging *students* in discussions, it is possible for them to gain experience with various models in chemistry education. It is, however, essential to pay attention in education to an adequate context in which this is possible.

3.6.2 Views on corpuscular models in chemistry education

The main question concerns learning and teaching how to work with models in chemistry education. By using the classification table, I tried to establish criteria to be applied when developing teaching material.

In order to formulate these, I combined the two-step description of the 'thesis' of reduction with the status of models and with the outcome of the analysis of the textbooks.

The first step of the thesis of reduction was linked to the acceptance of the hypothesis of corpuscular models and the second step to the use of these models. The status of corpuscular models was described as not being the reality and not being the conception of reality, but a tool designed for studying it.

I relate the first aspect of the status of the model, i.e. a model not being reality, to the first step of the thesis of reduction. I give three examples of the difficulties with models and reality in chemistry education.

1. With some types of models, such as for instance scale models, the model character is relatively easily recognisable, especially when the real thing is available to look at. However, as Keller remarks: the introduction to thinking in models is not simple because, as can often be seen in educational practice, models are interchanged with direct assertions about the reality (Keller, 1977, p.17). The results from the three textbooks on the acceptance of the hypothesis of corpuscular models show that measures should be taken to further the acceptance. It is difficult to distinguish between model and reality for students not yet proficient in thinking in terms of models.

2. A second point to be brought forward with regard to the potential confusion of corpuscular models and reality is how a molecule is defined. This is one of the reasons for the *minima naturalia* dilemma. Two definitions of a molecule are common in chemistry education: a molecule is the smallest particle of a substance; and, a molecule is a group/cluster of atoms. In some introductory chemistry courses the molecule is introduced before the atoms, and in that case the substance definition of the molecule is used. Sometimes this definition is extended as follows: the smallest part of the substance that retains the properties of that substance. Even without the extension, it is evident that the connotations of the word 'substance' enhance the idea of a molecule as something 'real', whereas in most educational situations it should be regarded as a corpuscular model.

3. Another stumbling block on the road to accepting models is the interchange of a picture of the model for the picture of the real thing. With the modern visualisation technologies it is very difficult to make a distinction between a figure generated by molecular modelling or a picture made with atomic force microscopy. In the next chapter I shall discuss aspects of the distinction between pictures of reality and pictures of models.

My conclusion is that to prevent students encountering difficulties in working with models, the first step of the thesis of reduction, i.e. the acceptance of models, *must be dealt with adequately in chemistry education, especially in the earlier stages*. (The same is applicable for physics education, cf. Vollebregt, 1993).

Secondly, I look at the aspect of a model not being the object and I relate this to the second step of the 'thesis of reduction', the use of models.

In the introductory paragraphs of the textbooks, the scientific method or scientific practice is briefly mentioned. However, in the subsequent treatment of chemical bonding minimal attention or none at all is paid to the hypothetical or model aspects of descriptions of chemical bonding. Chemical bonding in these textbooks appears as a real thing and not an idea in a theoretical sense. The distinction between model and object is not visible, and the model and the object are seemingly the same. Therefore, the use of models cannot be made clear, nor why it is useful to work with them. In the above-mentioned textbooks, step two of the thesis of reduction on the use of models is not applicable to the descriptions of chemical bonding.

From these answers and considerations, I distilled the following criteria for designing teaching material:

Preferably, students should design and use their own models for the experiments and theories under consideration. However, this is not always applicable in school practice. A restriction is that the canonical models of the corpuscular nature of matter and of chemical bonding are prescribed and not open to alteration. In the next chapter, I will present the results of a search for an alternative approach to circumvent around the limitations of the canonical models.

Students should have an opportunity to discuss models in the classroom, preferably with various models simultaneously available. Students should be stimulated to take an active part in a decision-making process on the advantages or disadvantages of various models. In doing so they will encounter the different contexts and realise the different meanings in these contexts. In this view, a simplified form of the pluralistic conception of science is suggested. Moreover, the idea of relativeness of the models will become clear through the discussions and this will help students remember that they are dealing with models and not with pictures of reality or substitutes for abstract objects. In order to prevent molecular shape and chemical bonding to be real things, students should have to go back to properties of substances and reactions.

The question to be answered in this part of the educational analysis was how can students acquire insight into models and how to use them. Since the models to be taught in chemistry are canonical models, students cannot develop and design their own models. However, through a simultaneous approach by introducing various models and providing opportunities to discuss and comment on these models and their applicability, students can come to an understanding of the relativeness of models. Therefore, the question to be answered in the educational experiment of the research project on chemical bonding is: *How can students gain an understanding of the relativeness of models in the context of chemical bonding?*

4 Educational Analysis and Educational Experiment

In the previous chapters I reported on the educational analysis of chemical bonding. The educational analysis was the first aim of the research project. The second aim was to develop an educational structure for chemical bonding. To achieve this aim I carried out educational experiments. Such experiments consist of designing an educational text and using it in a cyclic procedure of testing, evaluating and adjusting. It is expected that this cyclic procedure will yield a possible educational structure. Reports on the educational experiments, in particular the design of the educational text, are given in this chapter and subsequent chapters of the thesis.

In Section 4.1 I discuss the function of the educational experiment and, in particular, the educational text designed in the research project on chemical bonding, with regard to the significance of educational texts in two different research approaches: i.e. concept developmental research and education developmental research. Both approaches are adopted in research programmes at the Centre of Science and Mathematics Education at Utrecht University. Furthermore, as the meaning of concepts is context-dependent and this dependency needs to be taken into account when designing educational texts, I introduce two terms: decontextualizing and recontextualizing. *Decontextualizing* is the process of analyzing and selecting specific chemical concepts and procedures from chemistry practice for educational purposes. *Recontextualizing* is the process of designing an educational text with contexts in which the chosen chemical concepts and procedures are meaningful.

In Section 4.2 I present the reasons for choosing the molecular structure theory to replace the 'first principle' approach.

The choice of structural formulae, reported on in Section 4.3, is discussed in the framework of teaching the idea of the relativeness of models. The purpose is to overcome the restrictions of working with canonical models.

In Section 4.4, I continue the educational analysis by looking into aspects of scientific practice: first, to describe a view of scientific practice and to argue how stable enquiry in science might be regarded as fluid enquiry in education (cf. Schwab, 1964), and, secondly, to show how hints for writing educational texts may be found in reports on writing scientific texts and historical narratives. The designed text should offer students the opportunity to experience the process of 'creating knowledge' in chemistry.

4.1 Developing Educational Texts and Contexts

In this section I start by discussing the function of the educational experiment with regard to the educational analysis and the educational structure presented in this thesis.

According to Van Driel (1990, p.19) an educational text has a *function* in an educational experiment intended for research into concept development. In educational research aiming to develop an educational structure for the concepts in question, the educational text designed is not an objective in itself.

The research project I report on in this thesis is, on the one hand, part of a research programme *on concept development*. On the other hand, as the project developed from the revision of a schoolbook (cf. Chapter 1), the proposal for this revised version might be regarded as the starting point of *education developmental research*. I come to this conclusion because I see several similarities between the development and design of the educational texts in this thesis and the development of texts in education developmental research as described by Gravemeijer (1994a, 1994b). I will discuss these similarities in the function of the educational text in both research programmes with regard to either concept developmental research or education developmental research.

According to Gravemeijer, three main categories on educational research may be distinguished: research aiming at *explaining, understanding, and creating*. Explaining is seen in terms of causal relations between variables, and understanding as "making sense of what is going on" (Gravemeijer, 1994b, p.11; cf. Van Keulen, 1995). Education developmental research belongs to the third category. This is interpreted in the framework of realistic mathematics education as *research 'to lay foundations' prior to developing ('creating') education*. Education developmental research yields educational material or prototype material (units, curricula) as its educational result, and the underlying local educational theories and the account thereof, as its research results (Gravemeijer, 1994a, p.66).

The work performed in the small scale project (cf. Chapter 1) and subsequently in the educational analysis of the research project (cf. Chapters 2 and 3) can be regarded, in my view, as explorative research prior to developing education on chemical bonding. An educational text is the educational result. As the aim of the research project on chemical bonding is to develop an educational structure, this educational structure might be regarded as the research result, i.e. a local theory.

The choice of a starting point for developmental research is, according to Gravemeijer (1994b, p.171), a general principle of realistic theory forming. This choice is "a starting point that lies in practice and in theories of practice". In my view, although the starting point of the small scale project was in a practice, *viz.* the practice of school chemistry, the starting point might not be in accordance with the above-mentioned principle. First, the aim of the research project of chemical bonding is not theory forming as conceived in realistic mathematics education. And, secondly, the educational analysis led me to change the starting point when looking into chemistry practices beyond school chemistry.

The starting point of the educational analysis shows similarity to choices made by Goedhart when he decided not to use a generally applicable theory on learning and

teaching but declared his preference, first for describing the process of teaching and learning as practised in an educational situation, and secondly, for including in this process the discussion of the chemistry content (Goedhart, 1990, p.91). I consider this preference to fit in with the educational analysis presented in previous chapters of this thesis, and with the procedures I followed for the educational experiment.

Looking at the chemistry practice is considered to offer valuable information with respect to choosing the concepts and procedures to be included in the educational text. *However, when the chemistry content is brought up for discussion, the educational analysis is not a 'closed chapter' and will have to be continued during the educational experiment.*

In order to describe the development of the educational text on chemical bonding I will discuss the main points by answering the following questions (cf. Gravemeijer, 1994a, p.69): *a.* where do the ideas and criteria come from; *b.* which procedures are used; *c.* which criteria are used for adjustments to the educational text.

a. The results of the educational analysis are the main source of ideas and criteria for the educational text. For instance, a chemical approach is considered appropriate when looking at theoretical topics such as chemical bonding, also when this is an approach starting from the substance itself. Another result is the preference for a simultaneous-model approach. This is formulated as teaching the idea of the relativity of models. However, some ideas have to be ruled out because of limiting factors, such as the ability of the students, their previously acquired knowledge and other factors related to the school environment. Furthermore, no ideas are yet formulated on *how* to design the educational text. This may perhaps require further educational analysis.

b. The procedure used in developing and designing the educational text for an educational experiment contains the following points:

- a first version of the educational text is designed using ideas and criteria drawn from the educational analysis and elsewhere;
- the text is tested on small scale in classrooms, and research material, i.e. observation notes, tape recorded discussions and written answers and reports, is collected;
- the research material is analyzed, adjustments are considered and further educational analysis may have to be carried out; preliminary thoughts on the educational structure are formulated;
- the second version of the educational text is designed;
- this second version is used in the classroom, etc.

This cyclic procedure is a common feature in concept developmental research as well as in education developmental research in the Centre of Science and Mathematics Education (see, for instance: Goedhart, 1990; Elzenga, 1991; Roebertsen, Voogt and Waarlo, 1993; Gravemeijer, 1994b; cf. Van Keulen, 1995; Klaassen, 1995).

c. An educational text might show considerably less coherence than intended when first tested in an educational situation. In order to adjust and improve an educational text, criteria are needed. Like the designing criteria, other criteria for adapting the text to fit the classroom situation can also be drawn from the educational analysis. In the analysis of three textbooks in Chapter 3, I look at the use of different models by distinguishing different contexts. Lack of coherence between the model of the free atom and the model of the Lewis atom is pointed out by using what I call an energy context and a distance context.

This approach i.e. *looking into 'differences in contexts'*, could well be a productive approach to the analysis, evaluation and adjustment of an educational text as well (cf. Goedhart, 1990, p.90).

Developing an educational text implies that choices have to be made, for instance, when selecting concepts from the chemistry context. When a concept is selected, it is removed from the context in which it is meaningful. Concepts outside their context keep their meaning among those who are familiar with this context. However, this is not the case in education, when students are not acquainted with either the concepts or their context.

When teaching concepts, the aim should be not only that students can reproduce the concepts, but that they can work with them in a meaningful way in a chemistry context.

Therefore, the objective in education is to maintain meanings of concepts in the educational material as far as possible.

This implies that a new context must be built in the educational text being designed, in such a way that the meaning of a concept in the original context is preserved by and large in the new context.

I call the isolating of a concept from the original context, decontextualizing that concept; and the building-up of a new, adequate context, recontextualizing it.

Designing an educational text involves both decontextualization and recontextualization of concepts.

Educational analysis is relevant for analyzing concepts and procedures in the framework of concept developmental research. With regard to decontextualizing these concepts and procedures, educational analysis has to be carried out to *select* appropriate concepts and procedures for the educational text to be designed. When the educational text needs to be adjusted for another round of testing, educational analysis will certainly be needed again during the adjustment process. Looking for criteria for recontextualizing concepts, on the other hand, may not only provide guidelines for writing and describing an educational text, but also useful pointers in the search for the educational structure of the concepts.

4.2 The Chemistry Context of the Molecular Structure Theory

Looking into the relationship between the chemistry and physics contexts I conclude that a 'first principle' approach to chemical bonding is not a compulsory part of the curriculum. Therefore, the question is whether there is a suitable *chemical* theory that covers chemical bonding.

I use four descriptions found in the practice of chemistry in order to identify such a theory, i.e. the *molecular structure theory*.

- The first of these descriptions is taken from a lecture given at the eleventh International Conference on Chemistry Education held in York in 1991. P. Koelewijn, division manager of an industrial laboratory, lectured on the search for alternatives to chlorofluorocarbons (cf. Vandichel and Appleyard, 1990). I learned from her lecture that the methods of working did not include searching for a solution to the problem from 'first principles'. Working in a commercial organisation and under the pressure of time apparently does not allow time for much theorizing. It appeared that a combination is used of experience acquired in previous chemical research, creativity and intuitive approaches, and *a knowledge of molecular structures and the related chemical and physical properties of substances*.

- The second description found in chemical historical practice is from an article by Nye (1993a) on "philosophies of chemistry". She points out differences between chemists and physicists with regard to their methods of working:

"Chemists have always been closer to experimental work, more thoroughly involved in the laboratory than natural philosophers, and less satisfied with idealizations of phenomena." (Nye, 1993a, p.5)

and:

"The methods of the chemist and the physicist differ. The physicist takes a small number of measurements, works out an equation or a model following the laws close to the classical mechanics or electromagnetism, and arrives at a more complex model, which allows calculation of the unknown. The chemist follows a method that is "convergent rather than divergent", a method that is less exact and involves much more numerous data, much of it not metrical in character." (Nye, 1993a, p.18. See also, Lewis, 1926, p.169)

Chemists sometimes seem to prefer pictorial theories that have been known for a long time:

"(...) employing the static structural and stereochemical images of late nineteenth century chemistry (...)"

"the daily work of organic chemistry is best served by the old pictorial theories" (Nye, 1993a, p.18)

An example of the pictorial theories mentioned here is the geometrical structure theory. According to Nye, history shows that *chemistry has developed at least one theory of its own, i.e., the molecular structure theory* (cf. Nye, 1993b).

- The third description shows how organic chemists in chemical practice work with the molecular structure theory.

"This classical mechanistic view of reality accepts that once we know how individual building blocks behave, we can determine how a collection of building blocks will behave. A good example is the study of how organic substances react chemically. Organic chemists have built up a body of experience so they know how groups of atoms - the methyl group CH_3 , the acetyl group CH_3CO , the phenyl group C_6H_5 , and so on - react. They can predict successfully how molecules containing these groups behave, and can design strategies to synthesise new substances." (Woolley, 1988, p.54)

The approach might be regarded as a reductionistic approach since complicated phenomena are explained and predicted by more simple subsystems. The quotation is, nevertheless, relevant to the search for a chemical theory for several reasons. First, it concerns the practice of chemistry and what chemists study. Therefore, it fits into the chemistry context of theories and phenomena. Secondly, the discipline is that of organic chemistry. In this discipline the structure concept coincides broadly with the molecular structure concept. I interpret the quotation as an example of chemical practice *of describing, explaining and predicting, using the relation between properties and structures.*

- The fourth description is by Weininger who looks at the structure theory as he outlines the molecular structure concept developed according to classical (nineteenth century) conceptions before and parallel to modern quantum theoretical conceptions. In my interpretation of his reasoning, mutual influences of quantum theories and classical molecular properties on each other are unavoidable, but:

"The concept of molecular structure is so central to modern chemistry that its status is now essentially that of an axiom. It is a uniquely powerful tool not only for rationalizing an enormous number of known chemical phenomena but also for predicting the outcome of chemical interactions not yet observed." (Weininger, 1984, p.939)

I gathered these descriptions and quotations in order to demonstrate the existence of a specific chemical theory, *viz.* the molecular structure theory.

Van der Vet (1989) states that the molecular structure theory cannot be described by just a few postulates but that an underlying unity can be discerned. "This unity is brought about by a shared reservoir of chemical compounds represented in a way that is recognized by every subdiscipline" (Van der Vet, 1989, p.18)¹. I doubt whether this is applicable for all subdisciplines of chemistry but I agree with him as it regards organic chemistry, at least.

¹ "Die eenheid wordt bewerkstelligd door een gedeeld reservoir van chemische verbindingen, die op een in alle subdisciplines herkenbare manier beschreven wordt." (Van der Vet, 1989, p.18)

I summarize Van der Vet's description of the structure theory (Van der Vet, 1989, p.20-24) as follows:

The structure theory can best be understood as a network consisting of layers with links within and between the layers.

- The first layer is the macroscopic layer of observed substances and chemical reactions;

- The second layer can be characterized by means of the concepts 'element' and 'compound'. In this layer, these concepts can be regarded as theoretical but not corpuscular;

- Atoms and molecules belong to the third layer, the microscopic layer (or what I prefer to call the corpuscular layer).

A fourth layer in the network might be that of quantum chemistry. However, the linkage between this layer and the others is regarded by Van der Vet as controversial and complex and I agree with him (see Chapter 2).

New developments of a theoretical or experimental nature may influence the network. Concepts employed up to that time do not need to be removed from the network but can continue to exist next to newly introduced concepts or be given a new, additional, meaning. Van der Vet describes the function of the network as that of organizing.

With regard to chemical bonding, covalent bonding is covered by the molecular structure theory in the description by Van der Vet (1989, p.24). In the third layer, a covalent bond is interpreted as a bonding electron pair depicted by a dash between two element symbols. If according to contemporary physics a dash is a naive description of a chemical bond, this has not led to doing away with the dashes in the framework of the molecular structure theory (Van der Vet, 1989, p.24). I gather from his arguments that the molecular structure theory has its own place in the foundations of chemistry.

From the foregoing I conclude that the molecular structure theory is a genuine chemical theory. *Therefore I consider it legitimate to select this theory instead of a theory of atomic structure and to use this theory as a starting point for developing an educational text on chemical bonding.*

In a pluralistic conception of science, quantum chemistry is one of the theories that could and should have a place in chemistry education, assuming a way can be found to surmount the conceptual difficulties. However, in chemistry education, it should be preceded by the molecular structure theory.

It could be regarded as a disadvantage that the molecular structure theory does not cover the whole of chemistry, but since it does cover organic chemistry, and also biochemistry, pharmacology and even polymer chemistry, and both scientific and industrial applications, the field is extensive enough for the purpose intended.

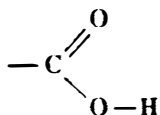
Part of the chemistry context is working with substances in laboratories. Chemical experiments play an important part in chemical theories, especially the relations

between properties and structure. Therefore, in chemical education, experiments are needed not just as an illustration but as an integral part of the development of a theory. If experiments are not possible because of financial or technical restrictions, it is important, in my view, to use descriptions of experiments whenever possible and to work by 'starting from-the-substance'. Great care should be taken to ensure that the students do not see a substance merely as an illustration of a structural formula. On the contrary, a structural formula should be seen as a way of representing properties of a substance.

The success of the molecular structure theory lies in the application of structure-property relations, in the explanation of properties of substances and their reactions, and in predicting new reactions and new substances (cf. Van Keulen, 1995, p.88).

Properties of substances are represented in molecular structural formulae, and these formulae are used to communicate about properties of these substances.

Communication in chemistry takes place not only through words, but above all by means of element symbols and drawings (see 'pictorial', cf. Nye, 1993a, p.18). And this belongs to experience with macro-micro relationships. In the practice of organic chemistry, for instance, the representation of the carboxylic group COOH is the representation of a set of properties of a substance. The element symbols indicate the composition of this group, i.e., carbon, oxygen and hydrogen. The sequence of the four letters comprises the representation of acidic properties by the position of the H in COOH, e.g. COHO would not be recognized as representing acidic properties. Furthermore, drawing the carboxylic group as



in a structural formula refers to a spatial structure for this group. This may be useful in explaining or predicting reactions, such as substitution or condensation.

These representations of the properties of substances, including reaction possibilities, are useful for communication among chemists and therefore should also have a place in chemistry education. *The representations of properties and the meaning of structural formulae are of fundamental importance in an educational text on chemical bonding.*

In the next section I examine the representation of properties of substances in the structural formula and the relation of these representations to models of molecules of these substances.

4.3 Molecular Models and Structural Formulae

The choice of the molecular structure theory for designing an educational text implies the choice of molecules as the main type of corpuscles within this theory. The two-step 'thesis' of reduction (acceptance and use of models) has to be taken into account with regard to the recognition of the molecules as models and to the functioning of the molecular models.

The molecular structure theory implies that molecules play the leading role, and therefore that structural formulae are important. The apparent simplicity of structural formulae is deceptive, in the sense that their meaning is at least twofold. On the one hand, they include aspects of corpuscular models, i.e., molecules, and on the other hand they represent macroscopic properties of substances.

In this section I come back to some aspects of models, specifying these with regard to corpuscular models. The first step of the thesis of reduction, i.e., acceptance of the hypothesis of corpuscular models, has become more complicated through recent developments in the use of microscopic techniques. Visualization by means of molecular modelling techniques make things even more complicated in this respect. As the limits of what can be perceived are extended the dividing lines between a picture of an object and a picture of a model of that object become less clear (4.3.1).

I discuss the assumption that the necessity for correspondence between object and model also applies to the model aspects of the structural formulae (4.3.2). Subsequently, I discuss how structural formulae imply the idea of relativity of models (4.3.3) and how these can be used for teaching this idea in the classroom (4.3.4).

4.3.1 *Shifting the limits of perception*

Molecules and atoms regarded as real or conceivable building blocks of matter (particles or corpuscles) are so extremely small that they can only be observed indirectly, using special equipment. Development of methods and devices for observing and registration, such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM), has resulted in 'pictures' of molecules and atoms. The results are often interpreted, in newspapers for instance, as the final proof that atoms and molecules really exist. A specific shape visible in a picture strongly suggests the presence of a specific molecule, especially when the shape of that molecule is known from models.

Editing the processed pictures into a video presentation creates the impression that what the viewer sees is the real movement of real particles, and that a chemical reaction can be observed on a molecular scale. An impressive video presentation of AFM experiments was shown by W. Heckl, from Munich University, when he lectured

on his experiments at the 1995 congress of NVON, the Netherlands Association for Science Education (cf. Leferink, 1995, p.228).

The AFM experiment was performed with a compound whose structural formula is known, and the space-filling material models. My interpretation after seeing the video presentation is as follows.

In the moving spots, i.e. molecules with atoms, and in the changing shades of grey, electron densities, I 'see' a chemical reaction on molecular scale if I also assume that:

- a chemical reaction is the forming and breaking of bonds between atoms;
- processes where hydrogen bonds appear and disappear are chemical reactions;
- a bond is formed when electron density between two centres of atoms increases and the bond is broken when the electron density decreases;
- light grey shades in a certain position indicate a relatively high electron density; when the shade of gray is darker, the electron density is lower.

The list of assumptions indicates that interpreting what is seen, i.e. white, grey and black shades and shifts of spots, as molecules and hydrogen bonds forming and breaking is theory-led, and dependent on far more assumptions than those mentioned here.

Pictures published as results of scanning tunneling microscopy and atomic force microscopy experiments led to claims that the pictures prove clearly that molecules and atoms exist because they really can be seen. However, it should be realized that the 'proof' depends on the calculations, manipulations and assumptions that lie between the object and the resulting picture.

This is already quite an obstacle to grasping that a model is a model and not the thing itself. An even bigger obstacle can be found in the form of the beautiful images of *models* of molecules created with new visualization techniques such as computational molecular modelling. Pictures of small parts of matter (particles) and pictures of models of these parts (corpuscles) show such a degree of similarity that the distinction between object and model of the object seems to be lost. *The first step of accepting the hypothesis of corpuscular models is therefore more difficult to make.*

Of course, explanations of the above-mentioned advanced techniques themselves should not be included in an educational text on chemical bonding, but the resulting pictures can be used to illustrate shapes of molecules for instance.

I want to stress that AFM pictures are not pictures of a model because they are a result of manipulating experimental data. I repeat a quotation of Apostel which De Vos (1985) used to distinguish between pictures of an object and pictures of a model of an object:

"...any subject using a system A that is neither directly nor indirectly interacting with a system B, to obtain information about the system B, is using A as a model for B." (Apostel, 1960, p.160; italics by Apostel)

According to this statement, data or processed data obtained by measurement do not form a model of an object. This must be taken into account when interpreting pictures resulting from measurements and comparing them to pictures of models.

The pictures deriving from AFM experiments and computational molecular modelling are photographs or pictures on a screen, and it is difficult to distinguish between them. Of course it is possible to give information on the status of the pictures in captions or in accompanying texts. However, one must be aware that the 'direct impact' of a picture might have its effect on viewers when an interpretation of the picture is proposed or when the origin of the picture is discussed. The viewers' first impression and the intended interpretation of the picture might not be the same. The same general objection applies to figures and drawings, in addition to the special problems inherent in the process of visualizing information and interpreting the results (cf. Bastide, 1988, p.210). The figure of the potential energy curve discussed in Section 2.3 is an example.

4.3.2 Correspondence terms; structural formulae as molecular models

In Chapter 3 I mentioned the use of the correspondence characteristic to distinguish between two contexts, energy and distance (Section 3.6.1). In this section I look closer into correspondence, especially with regard to structural formulae as models. As mentioned before, a model should be simpler than what it represents (Section 3.3.1). However, it seems plausible that there must be a common basis if the model is to function in relation to phenomena and experiments, and also in terms of the theories involved.

Nagel suggests "that 'length', 'mass', and 'time' are the primitive terms of the theory and 'velocity' and 'kinetic energy' can be (...) defined on the basis of these primitives." (Nagel, 1961, p.102). According to Lind (1980, p.17), the fundamental concepts of classical theories are space, time, mass and force.

De Vos (1985, 1990) points out the educational practice of describing corpuscular models in terms of space, time, mass, energy and also electric charge:

"Using mass, space, time, energy and electric charge as elements in building a corpuscular model of matter means that these five phenomena themselves can never be explained by such a model. But the model can be useful in explaining other aspects like temperature, colour, conductivity, and the formation of chemical bonds." (De Vos, 1990, p.173)

Apart from the drawback of not being able to explain a phenomenon (or object), it is not easy to distinguish between a molecule as the smallest particle and a molecule as a corpuscular model when both seem to have the same mass and the same shape. This aspect of the minima naturalia dilemma might belong to the educational research objects of naive models, preconceptions, misconceptions, etc. However, my conclusion is that the cause for the dilemma lies beyond the framework of education. This is a

difficulty which must be dealt with when teaching models and here the idea of the relativity of models could be useful.

The five terms mentioned by De Vos are what I call correspondence terms. There are models in which one of the terms predominates. If, for instance, the focus is on spatial aspects of an object, I call the model of this object a spatial model, and the context in which these models function, the spatial or distance context (cf. Section 3.6.1).

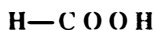
Structural formulae can also be seen as models because they share one of the aspects of corpuscular models. This can be recognized in the way the structural formulae are drawn in the notation of element symbols and dashes. The dashes can indicate distance, and since the proposals of Van't Hoff (1874), this can be interpreted as distance in a spatial sense. This corresponds to what De Vos calls 'space' and Nagel 'length'. Furthermore, the relative position of the atoms in the structural formulae can have a meaning corresponding to the position of atoms in a molecular model. Therefore the model aspect of structural formulae can be expressed in the correspondence term of length. The matching context is then the length context or distance context, since the dimension of this context is the same as the distance context which I have introduced and used in Chapter 1 and Chapter 3.

4.3.3 Structural formulae: representation of properties and molecular models

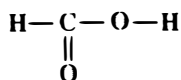
Structural formulae are also the shorthand notation of information on substances and reactions and therefore a means of communication in chemistry. In the quotation from Woolley in Section 4.2, an example is given of this. It shows that properties of substances are represented in structural formulae according to rules that belong to the "body of experience" of chemists. However, the use of structural formulae is complicated.

Various types of structural formulae can be used to represent the same substance, and each type of formula could reflect ideas of the chemical theories upon which they are based.

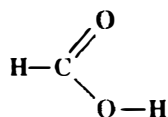
The structural formula of formic acid HCOOH might be drawn, for instance, as



or with rectangular angles as



or with angles resembling X-ray experiments:



Each of the drawings represents the elemental composition of formic acid. Each of the drawings has a specific position for the hydrogen atom that represents the acidic properties of formic acid. The rectangular drawing shows relative positions and bonds between the atoms, and this indicates how formic acid decomposes into carbon monoxide and water. However, this drawing is wrong in the spatial sense, and this is also the case, to a lesser extent, with the third drawing since the third dimension is not visualized.

In a structural formula, representations of the properties of a substance and models of the molecule are visualized.

In this thesis I focus on visualization as an aid to communication in the framework of canonical models. I discuss the usefulness of structural formulae in chemistry education as a means of communication, both as representing a substance and its properties and as a molecular model.

Referring to communication in chemistry, Habraken mentions the pictorial language of chemical structures:

"When chemists talk and think about chemistry, they do this in terms of chemical structures. It is as if the ability to see things pictorially is more highly developed in chemists than in the exponents of other disciplines. For a chemist, pictorial language is the most natural thing in the world." (Habraken, 1991, p.376)²

In her view, the pictorial language of chemistry is universal in the practice of chemistry and she refers to articles on chemical structures and pictorial communication by Hoffmann and Laszlo (1991) and Luisi and Thomas (1990).

I use statements from these two articles to discuss a proposal for using representations in the form of structural formulae in order to teach the relativity of models.

Luisi and Thomas (1990) say about pictorial language:

"Formal pictorial representation of a substance is essentially a form of modelling, a way to represent reality in a concise way on paper, but, with use, it has become more than this, it has become a way of thinking, and in chemistry, the dominant way of thinking. In operation, the pictographic molecular paradigm reduces the reality of a chemical compound to a visual representation of its apparent spatial form and exerts what is, in effect, pictorial reductionism." (Luisi and Thomas, 1990, p.67)

The title of their article is "The Pictographic Molecular Paradigm", where the meaning of pictographic includes the elements of symbolism and pictorialization.

² "Als het over chemie gaat, praten en denken chemici in chemische structuren. Het lijkt wel of het zintuig voor beelden bij chemici beter ontwikkeld is dan bij andere disciplines. Voor iemand die eenmaal scheikundige is geworden, is beeldtaal de gewoonste zaak van de wereld." (Habraken, 1991, p.376)

Hoffmann and Laszlo use similar expressions when they say "a chemical formula is a concise paraphrase, in a half-symbolic, half-ionic language ..." (Hoffmann and Laszlo, 1991, p.10).

They discuss seeing representations of molecules-as-reality as a way of thinking just as can be gathered from the quotation of Luisi and Thomas. This might possibly lead to similar difficulties as mentioned in the minima naturalia dilemma.

In both articles it is argued that working with pictographics is deeply embedded in the culture of chemists (Luisi and Thomas, 1990) and that it is a "shared code" (Hoffmann and Laszlo, 1991). The role of pictographics is to convey a great amount of information in a condensed form, for instance, to communicate about colour, solubility, chemical reactivity (Luisi and Thomas, 1990). It is a disadvantage that dynamics cannot be represented. But, as Nye pointed out, a curved arrow can represent displacements of electron pairs (Nye, 1993b, p.222). This is the case when structural formulae are used to communicate features of reaction mechanisms.

Because the information is condensed, structural formulae have several meanings, often represented in different forms, but in any case known by group consensus. A chemical formula is "at once a metaphor, a model (in the sense of a technical diagram), and a theoretical construct" (Hoffmann and Laszlo, 1991, p.10). Its use in a specific context will determine the meaning and the function.

Knowing different ways of representing a substance and knowing the various meanings of these representations is part of practising chemistry.

4.3.4 Teaching the relativity of structural formulae

The variety of meanings and representations makes it possible to present different representations side by side. It can be demonstrated to students that some representations are no longer adequate when new experimental data about a substance become available, and that therefore either the meaning of the representation has to be changed or the representation adapted.

In other words, the relativity of representations can be brought out in education by comparing the different representations of a substance and the various models of its molecules.

An educational unit designed to teach the idea of the relativity of models should offer students an opportunity to discuss a number of models and then to make well-reasoned choices. Students should always be made aware that various models are possible and that the choice of a model depends on its applicability and accessibility. The difficulty is that in normal educational practice, the freedom to create one's own models is almost non-existent because, as I argued in the previous chapter, current scientific theories and models (canonical or consensus) must be taught.

Although chemical formulae and structural formulae in particular have to be drawn in accordance with rules generally accepted by chemists, there is a certain degree of

freedom, allowing students to make choices. This creates opportunities to compare and discuss the applicability of the various representations.

A structural formula is a model of a molecule, but a structural formula also represents the properties of a substance: in this sense, the model aspect and the representational aspect might play conflicting roles. This could lead to the model becoming a minimum naturale, as for instance, when one hydrogen atom in the structural formula of formic acid is called an "acidic H".

As the condensed information about the substance seems to be very important in the thought and work processes of chemists such as Hoffmann and Laszlo and Luisi and Thomas, the question is whether the same applies to students. Which aspect is predominant for students? A student, reflecting on the relation between substance and structural formula, remarked that, in order to investigate a substance, first the structural formula must be known. Only then could one investigate whether the substance is soluble, or which reactions are possible. *The student did not realize that the condensed information has to be represented first before it can be used. Moreover, by wishing to start with the structural formula rather than from the substance, it might be concluded that the aspects of the structural formula as a model were not recognized either.* Consequently, this is another argument in favour of starting from the substance when designing an educational text.

Although this is only an example, it indicates that school chemistry has drifted away from chemical research practice and that the links between the two need to be reconsidered.

In the framework of decontextualizing concepts, the theory of molecular structure and the structural formulae with their function in communication about substances and reactions are suitable elements to be included in the educational text to be designed.

In the next section I look at the chemistry practice and chemical research in particular to find ideas for recontextualizing.

4.4 Building Contexts

In this section I discuss the criteria for defining suitable contexts in an educational text. Once concepts and procedures from chemistry practice have been selected as topics for the educational text, it is necessary to recontextualize them, i.e., to choose and build a context or combination of contexts which is as close as possible to chemistry practice. The practice selected for chemical bonding in pre-university education is the practice of chemistry as a science.

The main characteristic of the broad domain of chemistry practice, be it science, industry or society, is that it is a human effort. In the scientific practice of chemistry,

people talk and act as if they are engaged in acquiring chemical knowledge, i.e. as if they are occupied in a process, *the process of creating knowledge*.

Several authors point to the process aspects of acquiring knowledge:

"(...) science is a process of *constructing* bodies of *tentative* knowledge, of discovering *different* ways of making data coherent, and 'telling' about a given subject matter." (Schwab, 1964, p.35; Schwab's italics)

"Education that aims at developing students' scientific thinking, should involve them in a process of making and assessing knowledge. That is to say: such education should invite students to participate in a kind of productive learning activity that resembles the way scientists acquire knowledge. Only then does it make sense to talk about 'realistic' education." (Van Oers, 1988, p.124)³

These authors refer specifically to the practice of science. The choice of a practice as a context for the educational text is the choice for chemistry as a science. Therefore, the educational text should have process-like aspects reflecting the acquiring and creating of knowledge in chemistry as a science.

First, I look into the scientific procedure that is commonly used for textbooks (4.4.1). Then, I focus on how the 'creating' of knowledge can be taken into consideration in an educational text (4.4.2). Feasible rules for writing an educational text are derived by examining rules for writing scientific papers (4.4.3) and historical narratives (4.4.4).

4.4.1 Procedures in scientific practice

Many textbooks are written from an assumption, sometimes mentioned in the preface or in the text itself, that the scientific method is a stepwise procedure. In the textbooks I have discussed in Chapter 3, attention is paid to the scientific method. In one of the textbooks, ChemP, it is "the manner in which scientists proceed to solve a problem" and this procedure consists of six steps (ChemP, p.2-3, p.807). In the first volume of the series CHEMIE, a stepwise view of the scientific method is also presented (CHEMIE 3V/H, 1983, p.87). However, from my recollection of working in the laboratory (cf. Knorr-Cetina, 1981; Latour, 1988), the procedure is never as clear-cut nor are the steps as distinct as the textbooks seem to imply. I therefore agree with Schwab (1964) in his critical discussion of the stepwise procedure.

Schwab refers to the traditional textbook formulation of the scientific method as consisting of distinct steps, and he describes it as a sequence of five steps: noting

³ "Onderwijs dat de ontwikkeling van wetenschappelijk denken bij leerlingen beoogt, moet leerlingen betrekken in een proces waarin kennis wordt gemaakt en beoordeeld. Dat wil zeggen: dergelijk onderwijs moet leerlingen meenemen in een vorm van productieve leeractiviteit die analoog is aan de manier waarop wetenschappers kennis verwerven. Alleen in die gevallen mogen we zinvol spreken over 'realistisch' onderwijs." (Van Oers, 1988, p.124)

relevant data, forming hypotheses, planning a test, executing the plan, and drawing conclusions (Schwab, 1964, p.31-32).

Schwab compares the steps of the schoolbook version with situations in scientific practice. With regard to the first step, a very important question in practice is how to determine in what way data are relevant. He argues that a process of selection takes place in the use of experimental data, and that decisions must be made on whether to use or ignore findings. In Schwab's discourse, he describes the last step, the drawing of conclusions, as problematic because most scientific enquiries fail to produce a conclusion, whether this is taken to mean bringing something to a close, or in the sense that some truth has been found (Schwab, 1964, p.32). Furthermore, he argues that enquiries do not take place as isolated events, but that results are compared with the existing body of knowledge, and that different scientists may make different selections and comparisons.

After giving "a revised version of the schoolbook study of the short-term syntax of the sciences" Schwab describes what he calls the *short-term syntax*, or, the *syntax of stable enquiry*. Most scientific enquiries are conducted according to a pattern of stable enquiry, where the scientist knows what to do, what questions to ask and what parts of the substantive structure of the discipline to use (Schwab, 1964, p.38-39). When the principles which are part of the stable pattern are no longer taken for granted and become themselves a subject of enquiry, the syntax is changing to that of the *fluid enquiry* or *long-term enquiry*. Schwab calls this enquiry fluid because "matters are no longer fixed and stable in the science" (p.40-41). It is called long-term, because in the long term, some of the inconsistencies or incoherences connected with the stable enquiries are no longer ignored or explained away.

Four objectives of the fluid enquiry are:

"detection of the inadequacy of a conceptual structure, identification of its particular weaknesses, devising of replacements. (...)

Th(e) fourth objective consists of the political-rhetorical-scientific hard work of obtaining acceptance of a new conceptual scheme by one's fellow scientists." (Schwab, 1964, p.43)

The first three objectives can be seen as a process of selecting and decision-making, or a process of choosing and constructing. The fourth is a matter of discussion and communication among scientists.

With regard to this last objective, Schwab gives his four criteria which are often conflicting, for evaluating the acceptability of new structures: adequacy, interconnectivity, feasibility and continuity. They can be conflicting, for instance, when arguments for connecting proposed new structures to the existing structure of knowledge demand an extensive reformulation of the old body of knowledge, and feasibility and/or continuity could be called into question (Schwab, 1964, p.44).

4.4.2 *Acquiring knowledge and the syntax of fluid enquiry*

I discuss an interpretation of Schwab's description of scientific methods with regard to those aspects of the stable or the fluid enquiry that might be suitable for recontextualizing.

As I said before, the current schoolbook formulation of the scientific method resembles the syntax of stable enquiry. This seems plausible at first sight when one wants the students to experience how scientists normally acquire knowledge.

However, matters that are firmly established in the pattern of stable enquiry from a scientist's point of view, may not be self-evident to a student, for whom these things are not yet fixed or stable. Instead, I am inclined to see points in common between *the process of acquiring stable knowledge by students* and *the syntax of fluid enquiry in scientific practice*.

I now discuss the objectives of fluid enquiry in relation to criteria for the educational text.

The first objective of fluid enquiry, as mentioned above, is the detection of the inadequacy of an existing conceptual structure. A student, of course, cannot know whether a concept does or does not fit into the *common body of knowledge accepted by scientific consensus*. However, a student can, and from the point of view of learning as constructing indeed must become aware of whether a new concept does or does not fit into her or his *own body of knowledge acquired earlier* (cognitive conflict).

With regard to the second objective, some parts of detecting the weaknesses by reflecting can be done by the students themselves, but other parts have to be supervised by the teachers.

The third objective of fluid enquiry, devising replacements, asks for creative insights and imagination. These aspects should be stimulated as students learn how scientists work or how to be a scientist. In science, the answers to questions are not known; on the other hand, students still working to acquire the common body of scientific knowledge already known cannot create their own answers. If they try to do so, the answers have to be approved by the teacher. Students have to be guided to answers already known to science, but not yet known to them. Creative routes to 'discovering' the answers should be advantageous within the discipline.

Within the constraints of school practice, there are degrees of freedom with which the fourth objective of fluid enquiry can be achieved. This can be the case during discussions, when selections have to be made among information from various sources; when decisions have to be made as to which data are important and which data should be ignored; and, lastly, when explaining an idea or a point of view is not only useful to convince fellow students but also to convince oneself of a new principle or of another point of view.

That this convincing can be troublesome and the inherent uncertainty can be frustrating, is something common to both school and scientific practice. It is important

for students to be confident about what will be expected of them during assessments, and it is in this framework and not that of scientific practice that one should see the question commonly fired at teachers: "why don't you tell us how things really are?"

Interpretation of Schwab's analysis conveys the idea of the scientific practice of creating knowledge as a human endeavour and the objectives of fluid enquiry for designing an educational text. It does not, however, give rules or indications on how to design or write an educational text.

4.4.3 Procedures of scientific writing

Communication is important in scientific practice, and the written form is the usual form for reporting results. Scientists select and re-order the outcome of the daily laboratory work in order to write their papers. This is reflected in education. Most chemistry textbooks include prescriptions on how to make a lab report. I regard these rules in the same light as the schoolbook version of the scientific method, namely, that stating the rules of the procedure gives no insight into the characteristics of the process of scientific research.

Knorr-Cetina describes in her book "The Manufacture of Knowledge" how the results of the daily practice of science are reported in a scientific paper. In her analysis, the standard form of such a paper is characterized by

"a tame, tightly regulated flow of reason within a structure provided by page and paragraph." (Knorr-Cetina, 1981, p.98-99)

Her essay is important for my arguments for several reasons. First, in order to state a point of departure, she gives a description of the 'fabrication' of scientific products:

"Scientific results, including empirical data, have been characterised as first and foremost the result of a process of fabrication. Processes of fabrication involve chains of decisions and negotiations through which their outcomes are derived. Phrased differently, they require that selections be made." (Knorr-Cetina, 1981, p.5)

Both this approach to science and the point that selection plays an important role in the making of knowledge, are comparable to Schwab's view of the objectives of fluid enquiry.

Secondly, the aim of her essay is "to establish the symbolic, contextually contingent and constructive character of the scientific manufacture of knowledge" (p.16). The emphasis is on contexts in which selections and decisions take place:

"It is the context which orients, through the selections it promotes, the process of reconstruction and development." (Knorr-Cetina, 1981, p.11)

In the third place, and of high relevance, an important part of Knorr-Cetina's essay is about the process of converting outcomes of practical laboratory work into the stylised form of a scientific paper. She describes this conversion as *decontextualisation* and *recontextualisation*. She points out that "scientists themselves actually decon-

textualise the products of their work when they turn them into 'findings', 'reported' in the scientific paper" (p.47).

"If the scientific paper is a decontextualisation with respect to practical circumstances and local idiosyncrasies of scientific action, at the same time it provides the reader with a recontextualisation, found in the Introduction." (Knorr-Cetina, 1981, p.110)

The struggle, discussions, small victories, major mishaps, coincidences and daily events of laboratory life are deleted from the material gathered in practice and only the information that is thought to be relevant according to several, sometimes unwritten, rules is converted into a report acceptable for the scientific community. Knorr-Cetina successively discusses the various parts of a scientific paper and discerns that different rules seem to be applicable for each part. Fellow scientists know the written and unwritten rules because of the communal nature of scientific practice. They know how to read between the lines or how to obtain the additional information elsewhere. In any case, they know that the written information is not to be taken at face value but that it needs to be interpreted, and that experimental data should be verified to see whether they can be reproduced.

Knorr-Cetina calls the conversion process a double mode of production: the *instrumental* mode of production which gives the laboratory results in a decontextualized form, and the *literary* mode of production which in the published paper offers the recontextualized form (p.130). Another description of the two modes is more relevant for my purpose: with the first mode I associate "sequential contingency" (p.107) which I interpret as a series of concepts in a certain order. The literary mode is mentioned earlier by Knorr-Cetina as a literary strategy that is commonly used in scientific papers with a language that is "ostentatiously neutral" and that is further characterised by the use of simplistic language, the passive voice and separation of 'information' from 'interpretation' (p.95). In a scientific paper a choice has been made of the sequence of the concepts and of the literary form in which the concepts are incorporated. When 'strangers in the field' are confronted with the texts there is a risk of misrepresentations and misunderstanding. This does not imply that scientific texts or extracts from them are not suitable for students; it might be preferable to include them in the educational texts. But, I do not consider the format of the scientific paper itself to be an appropriate design criterion for an educational text.

As I was looking for ideas for recontextualizing, the interpretation of the foregoing 'data' yields two criteria: a 'sequential contingency' of the chosen concepts and some kind of literary strategy for the writing of an educational text.

4.4.4 *Historiography and educational narrative*

Historiography could be a good source of guidelines for designing an educational text, because, in my view, historians must be used to handling facts and events 'that cannot

be changed'. The question is how historians cope with information from the past, accepting that the past can not be relived.

According to Ankersmit, a distinction can be made between 'historical research' and 'the narrative writing of history'.

"When the historian does his historical research we can compare him with a detective: he wants to know what actually happened, who did or wrote what, how texts should be interpreted and so on." (Ankersmit, 1981, p.8)

The historian is, however, more than a 'fact-finder' in the view of Ankersmit, because:

"Learning to know the facts is only a preliminary phase in the task he sets himself. For his real problem is how to integrate these facts into a consistent historical narrative. (...), this is what I called the 'narrative writing of history'." (Ankersmit, 1981, p.8)

With regard to facts, the dividing line between historical research and narrative writing is not sharply drawn, because facts are looked for and described within a specific framework of narrative interpretation. For some historians, the question is what might be the most acceptable representation or synopsis of parts of the past (Ankersmit, 1981, p.8-9).

In an educational text, the facts to be incorporated need not be facts from the past, they can be facts from the present as well. Is it possible to integrate these facts 'that cannot be changed' into a consistent narrative for educational purposes?

To answer this question, I try to interpret some of Ankersmit's arguments. When he writes that statements should describe the past and that "by means of these statements some 'image' or 'picture' of the past (...) is constructed" (Ankersmit, 1981, p.214), I notice that in history writing too, a constructivist approach can be found. Of the two functions of statements, the first, 'describing the past', is the easiest to interpret, because I can relate this function to comments by Ankersmit on a linear, linguistic approach and because I can link this approach and the 'describing of the past' to the sequential contingency of Knorr-Cetina. The linear, linguistic approach will result in an intelligible piece of language, - and Ankersmit gives chemical treatises as examples of such texts (Ankersmit, 1981, p.214) - but it is not sufficient for the narrative writing of history. Then attention must be paid to what he calls the 'constructive' aspects of the narrative discourse, i.e. the second function of a statement. This function I find difficult to interpret because the discussion of this function is closely associated with historical practice. The idea of 'image' or 'picture' is introduced with an example of an 'image' as a 'thesis on the past' or as a *guiding principle* in narrative writing (Ankersmit, 1981, p.102) and I recollect such an image-like guiding principle when writing the first version of an experimental unit, i.e., how can one know the structural formula of a newly found substance. By associating 'a point of view', 'image' or 'picture' of the past and a global approach rather than linear approach, I arrive at the idea of a coordinating or *global context*.

I interpret these findings with regard to ideas on recontextualization as follows: *From a strictly chemical point of view, a linear linguistic approach might be adequate for a chemical treatise because of the familiarity of the chemical community with the rules. However, for educational purposes, a global approach seems to be more relevant, for instance, in the form of a narrative that includes the chemical information in a sequential contingency, but that is written with a guiding principle and set in a global context.*

When building contexts for the sequential contingency of chemical concepts and skills chosen from chemistry practice, the specific educational targets determine which guiding principles and which global contexts might be appropriate to achieve those aims.

5 Getting Acquainted: an educational experiment

In this chapter I report on the educational experiment conducted with an educational text as part of a cyclic procedure of development, testing, evaluating and adjusting. I use the terminology introduced in Chapter 4 to describe how the educational text was designed and written. Since the assignments appeared to be relevant as they offer opportunities for communication and for gathering research material, I focus on the assignments in the educational text and the titration assignment in particular.

The educational text is entitled 'Kennis Maken'. This title has a double meaning: 'Getting Acquainted', and 'Making or Creating Knowledge'. Both seem to be appropriate for a text dealing with the creation of knowledge as a human endeavour. The first version of the educational text is available only in Dutch; the second version which has been adapted as part of the cyclic procedure, is included in the Appendix.

In Section 5.1, results from the educational analysis in the foregoing chapters are discussed with a view to the selection of concepts and procedures for writing the educational text. Sections 5.2 and 5.3 deal with the chemistry aspects and the narrative format of the educational text respectively. The following sections, 5.4 and 5.5, concern the role of assignments and the results of experimenting with the text in a classroom. In the concluding section, 5.6, I discuss the different contexts which can be distinguished in the titration experiment and I will discuss a sequence of contexts described on the basis of correspondence terms and with regard to a tentative educational structure for molecular chemical bonding.

5.1 The Educational Text

The educational text 'Kennis Maken' was designed and written after the small scale project of Hoofdstuk 10 was finished (cf. Chapter 1) and while a further educational analysis of chemical bonding was being carried out. Results from the educational analysis in Chapter 2 and 3 and further considerations reported in Chapter 4 provided arguments for rejecting the approach to chemical bonding based on a physical atom and potential energy context.

The ideas and criteria for 'Kennis Maken' were first formulated as a chemical, simultaneous-model and 'knowledge-creation' approach, using knowledge of chemical concepts and procedures and teaching experience to try and overcome the problem of the gap. The terminology introduced in the previous chapters enables me to discuss the ideas in 'Kennis Maken' and describe the objectives of the text designed. In the framework of the educational experiment, the text should enable students to acquire more insight into how to use models. *Acquiring insight into working with models means that teaching the relativity of models is the main idea for the educational text.*

The selection of appropriate concepts led to the notion of 'removing concepts from their context' i.e. the notion of *decontextualization*. Subsequently, I called the building up of new contexts around selected concepts in an educational framework *recontextualization*. In Section 4.4, I discussed several points to be considered with regard to recontextualization, for instance, discussions as a part of fluid enquiry, and three guidelines for an educational text, i.e., *guiding principle*, *sequential contingency* and *global context*. I will use these guidelines to describe the objectives, the content and the narrative of the educational text designed.

5.1.1 Objectives

I discuss three objectives for writing the educational text in relation to the guidelines for recontextualization.

1. With regard to teaching chemical bonding from a more chemical point of view, I explored the chemical background in Chapter 2 and Section 4.2. The objective for the educational text was: *to start from the composition and properties of a substance, to arrive at a way of representing them in the framework of the molecular structure theory.*

The criterion of starting from the substance itself can be called the guiding principle for recontextualization.

2. With regard to a simultaneous-model approach, I argued in the previous chapter that structural formulae contain aspects of models and that they can be used for teaching the relativity of models. Working with structural formulae belongs to the molecular structure theory. Using this theory will provide reasons for constructing new representations or for attributing new meanings to symbols in structural formulae. *The possibilities of various representations in a structural formula and also the use of structural formulae for communication make these formulae appropriate in the framework of the molecular structure theory.* The objective for the educational text, the molecular structure theory, provides the sequential contingency for recontextualization.

3. Students should learn to distinguish between contexts. Furthermore, they should become aware of the process of creating knowledge through discussions and decision-making. As I argued in Section 4.4.2 on fluid enquiry, this includes ascertaining the relevance of data, interpreting texts, and, in general, gaining experience of grappling with uncertainties.

In Chapter 3, I mentioned three methods of introducing models in education and I argued that using several models side by side most closely resembles scientific practice. *Discussing several models in various contexts and explaining the reason why it was decided to use them, could be a good way of imitating scientific practice in education.* The objective of dealing with the creation of knowledge as a human endeavour is the global context of the educational text.

In addition to these objectives, which were discussed in earlier sections, I considered two more issues relevant to designing the educational text: firstly, the input of recent developments in chemistry practice, and secondly, the restrictions of the school circumstances.

- By reflecting on chemistry education and looking beyond the bounds of 'normal' school chemistry, topics were identified from current chemical research which could be incorporated or at least considered for incorporation into an educational text on chemical bonding and molecular structure theory. Determination of crystal structure using electron density plots simulated with computer modelling was such a topic. Other topics could come from chemical industry, e.g. industrial applications of polymer chemistry. Ideally, the new educational text should also show how fascinating chemical research can be and should include 'beautiful' chemistry (cf. Minssen, 1986, and Minssen, Popp and De Vos, 1990).

- The objectives of the text are restricted by preconditions associated with the classroom situation in Year 13 (pre-university education), such as students' previous knowledge, the existing curriculum, the amount of time available, and the period available in the school year. As the educational text was designed initially to replace Hoofdstuk 10 (or parts of this chapter), the text was made to match the programme of the highest level of secondary education. This meant that the chemical knowledge which students could be assumed to have was set out in the exam syllabus (Eindexamen-programma, 1984).

5.1.2 Content

In the chemical approach chosen, a substance is the starting point of the journey from chemical composition to structural formula. The molecular structure theory is the basis of the educational text. This means that the focus is on the relationship between structure and properties of substances, the structure-property relation of substances.

The sequence in which topics are dealt with in the text is based on an interpretation of the molecular structure theory described by Van de Vet (1989), which is discussed in Section 4.2 of this thesis. Applying this theory to structure-property relations entails observing properties, representing them in formulae and using these formulae to describe, explain and/or predict properties. Therefore a structural formula must be attributed to each substance.

The following description of a procedure based on this theory gives a more detailed picture.

Suppose an unknown substance is observed in an organic chemistry experiment. In order to identify the substance, experiments are carried out. Qualitative and quantitative analysis yields the elementary composition of the substance and provides the first opportunity to represent the substance in an *empirical* formula. In the interpretation of the molecular structure theory, this is the transition from the macroscopic layer to the second layer of elements and compounds. In the second layer, the empirical formula is

to be considered in a non-corpuseular sense. The molar mass is then determined and the *molecular* formula can be written up. Depending on what knowledge has been acquired beforehand and how this knowledge has been assimilated, the molecular formula can be regarded as belonging to the second layer of elements and compounds (the term 'molar formula' would be appropriate), or the third layer of corpuscles, i.e. molecules and atoms (cf. Van der Vet, 1989).

The next step of depicting the substance in a *structural* formula could be performed using valencies and rules on how to work with valencies. If more than one structural formula are possible, a decision must be made, using properties already known or yet to be discovered, as to which structural formula is most appropriate to represent and depict the substance. *Therefore, a structural formula of a substance is worked out by using knowledge of several chemical and physical properties of that substance and by applying chemical rules to depict a molecule in pictographic form.*

Once a structural formula has been attributed to a substance, chemical research does not stop. The molecular structure now reflected in a structural formula, does more than just represent the properties of the substance which are already known; it also suggests additional properties and raises questions to be answered by further research. An interactive process now gets underway, involving describing and explaining properties by means of the structural formula, extending the meaning of the structural formula, predicting other properties and suggesting possible reactions.

The procedure in the *current* practice of chemistry more or less follows the procedure described above. Chemists working in scientific research and industrial laboratories use a combination of information from various sources, for instance: the 'origins' of the substance, various methods of analysis (mostly spectrometric) and the determination of the elemental composition "to establish identity and purity" (Heathcock, 1990, p.8A; cf. Van Dijk, Lugtenburg and Cornelisse, 1995, p. 1493-1494). Chemistry practice also shows that data from new measurements, information obtained by more advanced methods of analysis and new theoretical insights sometimes lead to other methods of representation or to attributing new meanings to existing representations.

The classroom situation in Year 13 places a limitation on the educational text: it must take account of the assumed knowledge of the students. Preferably the knowledge includes: the occurrence of bonded atoms, the values of electro- and covalencies, properties and structural formulae of simple organic compounds and concepts such as the hydrogen bond and vanderwaals forces. An overview of the previous knowledge with regard to chemical bonding is given in Section 1.1. This knowledge determines the choices of substances, preferably simple organic compounds. Simple organic substances in the school situation are substances with low molar mass, which consist of few elements. Another restriction in the school situation is the equipment available: the spectrometric methods of analysis widely used in chemistry today are not possible in most school laboratories.

A brief comment on the relationship between formula and corpuscle should be made here. As mentioned above, in the second layer of the molecular structure theory (elements and compounds), the empirical formula is considered in a non-corpuscular sense. However, students involved in the educational experiment had already been taught corpuscular interpretations of formulae long before the experiment started. Actually, students began to speculate about structures by using empirical formulae in a corpuscular sense. Trying to teach a non-corpuscular interpretation of molecular and structural formulae would therefore be unrealistic. Moreover, given the successes of the corpuscular research programme, such an approach would run the risk of alienating students from modern chemical research. For these reasons, a non-corpuscular interpretation of molecular and structural formulae is not pursued in this thesis.

5.1.3 Narrative

In Section 4.4 I went further into criteria for designing an educational text that reflects aspects of fluid enquiry, and I stressed the importance of communication as part of scientific practice. *Therefore, an educational text should offer opportunities for discussions on experiments, interpretation of information, reflection on the issues at hand and attempting to reach a consensus.* These aspects are taken into account in the assignments by attributing a dialogue function to the assignments.

The narrative format of the educational text is that of a biography of a substance and, at the same time, a story about getting to know more about a substance and about the process of creating knowledge. As can be seen from publications in journals and books, people gathered knowledge about the substance, and in doing so, they contributed to the growing body of knowledge about that substance. The two aspects, 'getting acquainted' and 'creating knowledge', are both reflected in the Dutch title of the unit, 'Kennis Maken'.

The narrative format might be compared to the way in which the Salters' Units are written. A storyline functions as the backbone of a unit which "provides the contexts within which chemical ideas are developed" (Burton, Holman, Pilling and Waddington, 1995, p.228). In a Salters' unit, new chemical concepts are introduced when this is regarded as necessary for understanding the story.

However, in 'Kennis Maken', *the aim is to examine structure-property relations in the global context of creating chemical knowledge as a human endeavour. The elaboration of the molecular structure theory as described above gives the successive steps in the narrative and, therefore, the sequential contingency.*

The subtitle of the educational text, 'the biography of a substance', points in the direction of starting from the substance itself, i.e. thinking with the substance in mind. The biography of a *substance* implies the existence of a substance, something material and tangible. *Thinking with the substance as the starting point is the guiding principle of the narrative.*

Not one single substance but a twin pair of substances, maleic acid and fumaric acid, was selected for the biography. In previous sections (cf. 4.4), I argued that the process

of creating knowledge implies making choices, deciding on the interpretation and using representations. The biography of one suitable substance should offer enough possibilities to explore this process. The biography of *two substances* with many similar properties will offer even more possibilities. The relation between the two substances allows for discussing essential aspects of the molecular structure theory in a convenient way (for instance, cis/trans isomerism, double bond, acidity).

The history of maleic acid and fumaric acid is a rich one, not only for science but also for the purposes of education (see Daecke, 1965; Snelders, 1974 and 1977; Meek, 1975; Van der Vet, 1989; Reiners, 1990).

Two aspects make it clear that the importance of these two substances, maleic acid and fumaric acid, in current chemistry also fits into the global context of people creating knowledge. First, while the structure of the two substances was a *topic of research* for chemists in the history of the development of structure theory, nowadays scientists use the two substances as a *model for research*, for instance, in the hydrogen bonds research programme (cf. Vanhouteghem, Van Alsenoy and Lenstra, 1991). Secondly, both substances are economically important as raw materials or as additives in a number of industrial processes and are therefore of interest to people in industry.

Selecting these two substances for the educational text does not imply that it is necessary for students to know everything about these two substances; they should be seen as *examples* of how a substance is investigated and how knowledge can be explored. They exemplify more general chemical concepts.

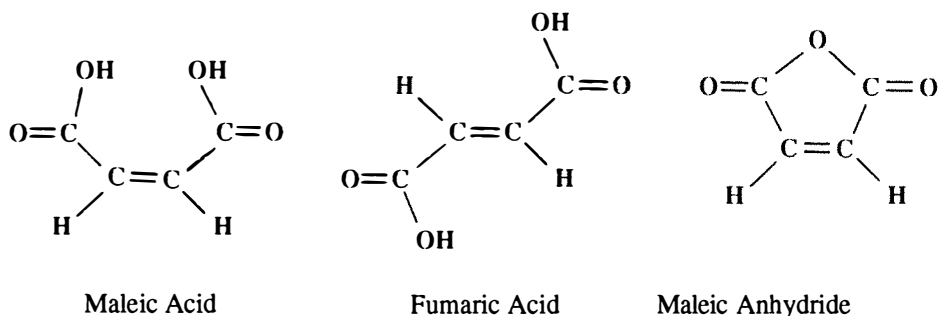
In the following two sections I describe the chemistry content and the narrative of the educational text in more detail.

5.2 The Substances and Their Reactions

In this section I summarize the biography of the two substances and some relevant properties. Firstly, the main properties of maleic acid and fumaric acid are given (5.2.1). Then I give the chemical information necessary for depicting the structural formulae in more detail (5.2.2). Subsequently, I go into the reactions used for elucidating further the relationship between structure and properties (5.2.3).

5.2.1 Properties of the substances

Both, maleic and fumaric acid are white crystalline substances with the molecular formula $C_4H_4O_4$. The systematic names are, respectively, *cis*-butenedioic acid and *trans*-butenedioic acid. Maleic anhydride, $C_4H_2O_3$, which is closely related to maleic acid, also plays a role in the educational text.



Several properties of these three substances which are relevant for the educational unit are included in the following table.

	Maleic Acid	Fumaric Acid	Maleic Anhydride
molecular weight*	116.07	116.07	98.06
melting point, °C	130-130.5	287	52.85
boiling point, °C	138 (dec.)	1651.7 subl.	202
heat of formation, kJ·mol ⁻¹	- 790	- 811	- 470
heat of combustion, kJ·mol ⁻¹	- 1358	- 1335	- 1390
solubility*			
water	very	slightly	(reacts)
ethanol	very	soluble	
K_{Z1} **	$1.42 \cdot 10^{-2}$	$9.30 \cdot 10^{-4}$	
pK_{Z1}	1.83	3.03	
K_{Z2} **	$8.57 \cdot 10^{-7}$	$3.62 \cdot 10^{-5}$	
pK_{Z2}	6.07	4.44	

The data marked with * are from Handbook of Chemistry and Physics (59th edition, 1978-1979) and with ** from Trivedi and Culbertson (1982). The remaining data are from Kirk-Othmer (1967) with the values for heat of formation and heat of combustion converted to SI units.

Maleic acid and fumaric acid and their derivatives are useful for various applications, as can be seen in the following overview.

Fumaric Acid

- ferrofumarate in tablets for anaemia
- food additive as acidulant
- raw material for the synthesis of aspartame

Maleic Acid and Maleic Anhydride

raw material for unsaturated polyesters

raw material for polyaddition polymers

(the polymers are used for manufacturing

shirt buttons, surfboards, furniture lacquer,

dishwashing detergent, etc., etc.)

raw material for specialties (Diels-Alder synthesis)

Fumaric acid is part of the tricarboxylic acid cycle (citric acid cycle). When fumaric acid reacts with water, a racemic mixture of both stereo-isomers of malic acid (2-hydroxy butanedioic acid) is formed. When specific enzymes are present the addition product is optically active malic acid.

Knowledge of the behaviour of fumaric acid is useful to understand polymerization reactions with maleic acid and maleic anhydride. In some polymerization reactions, e.g. copolymerization with styrene, the *cis* isomer (maleic acid) is converted into the *trans* structure in the polymer chain.

Maleic anhydride has some attractive properties for polymerization reactions: it reacts fast in the first step of the polymerization process; it can be added in a molten state because of its relatively low melting point.

The safety precautions required for the two acids are easy to meet, so they can be used in the classroom under normal conditions, except in experiments where they have to be heated. These must be executed in a fume cupboard because of the possible formation of maleic anhydride vapour.

5.2.2 *Substances and structural formulae*

The educational text enables students to work out the structural formulae of the substances selected in a series of assignments. The first step is to obtain the substances. This is performed in a fume cupboard by slowly heating some malic acid (2-hydroxy butanedioic acid) in a test tube in an oil bath while keeping the temperature below 200°C. Small white crystals of maleic acid appear halfway up the tube. Another white substance, fumaric acid, appears at the bottom of the tube. Students establish that an aqueous solution of maleic acid turns red with litmus, and produces a precipitate with a solution of barium hydroxide, but not with lime water.

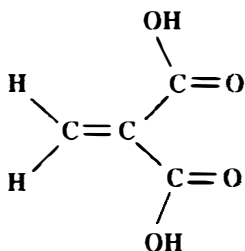
Qualitative elemental analysis is performed by heating a sample of maleic acid with an excess of CuO, using anhydrous copper sulphate and lime water to ascertain that the substance contains the elements hydrogen and carbon, respectively. The results of a quantitative analysis combined with assuming the element oxygen to be present and using modern values of the atomic weights will allow students to establish the empirical formula $(\text{CHO})_n$ for maleic acid.

Fumaric acid differs from maleic acid in its solubility in water (only slightly soluble) and does not give a precipitate with a solution of barium hydroxide. The results of the

qualitative and quantitative analysis are the same for maleic and fumaric acids. *Therefore, the two substances have the same empirical formula.*

To find out the value of n in the empirical formula a value of molar mass is determined by performing an acid-base titration. Such a value can be calculated from the results of the titration, since the amount of acid and the molarity of a sodium hydroxide solution are known. The acids are bivalent. Therefore, two suitable indicators are used, *viz.* methyl orange and phenolphthalein. Two points of equivalence of maleic acid are clearly observed during the titration. However, in the case of fumaric acid, the first point of equivalence is difficult to determine because of a gradual change in colour of the indicator, methyl orange. A gradual change of pH is observed when a titration curve is made using a pH meter. From these results the value of n in the empirical formula is calculated to be 2 or 4, but the conclusion is that $n = 4$, for both maleic and fumaric acids. *Thus, both substances have the same molecular formula, $C_4H_4O_4$.*

Structural formulae based on the above conclusion are drawn up in order to distinguish between the two acids. The knowledge that the substances are organic acids, plus previous knowledge of valencies and an understanding of simple organic acids can be used to conclude that *three structural formulae are possible*. In addition to the *cis* and *trans* isomers a third structure is drawn using all the information gathered: 1,1-ethenedicarboic acid. No evidence is available that this third product is formed during the heating of malic acid.



1,1-Ethenedicarboic Acid

Maleic acid and fumaric acid show the same addition reactions with a bromine solution, which is an indication for a double carbon bond in the structural formulae. When gently heated, only maleic acid reacts. Results of the elemental analysis of the reaction product show that maleic anhydride and water are formed. This points to a structural formula for maleic acid with the two carboxylic groups in the *cis* position. The structural formula with the *trans* position is for fumaric acid.

During the process of building up of the structural formulae, various properties are used, including the reaction properties of the substances. In the following I present a number of reactions with the substances in relation to the meanings of the representations of these reactions in the structural formulae.

5.2.3 Structural formulae and reactions

The two structural formulae are drawn up by making use of information from several reactions, such as the acid-base reaction and the formation of an anhydride. Once the formulae are known, more information on reactions leads either to changes in depicting the formulae, or to extending the meaning of the formulae. I call this '*adding layers of meaning*'.

In the next part of the educational text, a number of reactions are given for the two substances, and also for other substances. Each of these reactions has consequences for the representation of a property in the structural formula, and consequently for the meaning of the dashes and element symbols in the structural formulae.

1. The above-mentioned reaction with bromine is an addition reaction. The possibility of an addition reaction is usually represented by two or three dashes between the two element symbols in a structural formula.

2. Two dashes between two element symbols do not always mean an addition possibility at that position. For instance, in conjugated systems such as 1,3-butadiene, addition does not only occur at the double bond. The reaction of 1,3-butadiene with a small amount of bromine results in a 1,2- *and* a 1,4-dibromine addition product.

3. The alternating system of one and two dashes indicating a conjugated system as shown in the structural formulae of maleic acid and fumaric acid is not accompanied by specific reactions such as mentioned above. Data from crystallographic measurements show only very slight evidence or none at all of the properties of a conjugated system, such as specific bond lengths.

4. The double bond in both acids is not as rigid as normally assumed for a double bond. When a small amount of bromine is added to a concentrated aqueous solution of maleic acid and the reaction mixture is placed in sunlight or strong artificial light, a reaction takes place and fumaric acid precipitates (Bader, Braun and Göttel, 1972). In another experiment, the mechanism of this reaction is investigated and the results are compared with the other experiments with bromine. The results show that the double bond in maleic and fumaric acids does not indicate addition reactions only.

5. An extension of the meaning of a dash is that of an electron pair. Used together with the octet rule, a dash in a structural formula means either a bonding electron pair or a non-bonding electron pair. Reactions such as the formation of ammonium salts from ammonia and acids are represented by using a non-bonding electron pair on the nitrogen atom.

6. The difference in the acid-base reaction of both substances is explained by intramolecular hydrogen bonds. Intermolecular hydrogen bonds are used to explain the difference in melting point of the two substances. Hydrogen bonds are usually drawn with dotted lines.

The various meanings which are attributed to the dashes have consequences for the meaning of the element symbols in the structural formulae. I will go into this when discussing a tentative educational structure in Section 5.6.

I described progressing from the composition of a substance to building up structural formulae and subsequently adding layers of meaning to the dashes in these formulae. For this purpose, I used various concepts and procedures from the molecular structure theory and presented these concepts and procedures in a certain sequence: *I used the molecular structure theory to establish the sequential contingency of the narrative.*

5.3 A Narrative with Episodes

In this section I trace the biography of the substances from the point of view of how knowledge about these substances was acquired. The format of the educational text is a narrative in five episodes. Each episode is related to a person or rather to his or her publications about maleic acid and/or fumaric acid. From the first systematic description of the twin pair onwards, the difficulties of representing the two substances pictographically has fascinated generations of chemists. Therefore, an abundance of material is available. A selection was made from sources from recent times as well as from the history of chemistry.

In the narrative, the chronological order of a life story is followed. A person with a specific relevant publication is the focal point of each episode.

The five episodes of the narrative are sections in the educational text of 'Kennis Maken'. They present the following parts of the sequential contingency:

- a. from the substances to the molecular formula, and a first attempt to design a structural formula for both substances (5.3.1);
- b. from the molecular formula to the structural formula for each substance (5.3.2);
- c. extending the meaning of the structural formulae to 'save the valence rules' (5.3.3);
- d. extending the meaning of the structural formula with crystallographic data (5.3.4);
- e. the application of structure-property relations in present day chemistry and in school chemistry (5.3.5).

In this section I describe the publication at the centre of each episode, then I discuss the contribution this information could make to a decision-making process and I summarize the state of affairs regarding the structural formulae at the end of each episode in 'Kennis Maken'.

5.3.1 The Pelouze episode

The central publication in the first episode is a comprehensive article (Pelouze, 1834) on the investigation of the products of dry distillation of malic acid crystals (molecular formula $C_4H_6O_5$). Pelouze reports on the reaction conditions by which maleic acid and its isomer are formed in this reaction. By using apparatus and techniques designed by Liebig, Pelouze decides on the qualitative and quantitative elemental composition of the reaction products. A molar mass determination (in his words: "das Atomgewicht") enables him to give the molecular formula, $C_4H_4O_4$, for both substances. Pelouze

mentions that it was difficult to get "constanten Zahlen" (constant numbers) for some of his experimental results in his investigations with maleic acid. He became aware that interpreting data was difficult because maleic anhydride is formed when maleic acid is heated (Pelouze, 1834, p.271). He states that one must be prepared for events of this kind especially when determining melting and boiling points of organic compounds:

"(...) since, of all driving forces, heat seems to be the main agent causing atoms to build groups in various arrangements, on which isomerism is based." (Pelouze, 1834, p.271)¹

The first episode of the educational text comprises information on Pelouze's experiments with regard to the formation and properties of the products of heating malic acid. Not knowing which substance is formed means that no name is known either. Because the name maleic acid, given by Pelouze, is still in use today, it was decided to introduce imaginary names that would not give away too much too soon. Using the usual names could encourage students to look up information in Handbooks and the book of tables. The pseudonym chosen for maleic acid is 'Pelouze's acid', and fumaric acid is temporarily named 'moss acid'. This name was chosen because the acid can be isolated not only from extracts of *Fumaria officinalis*² but also from various kinds of moss.

Quotations from the article included in the educational text describe the substances and give data from the quantitative analysis. The determination of the molar mass which is needed to be able to draw up the molecular formula is performed by the students by means of an acid-base titration, as mentioned in Section 5.2.2. This was done for two reasons: to combine findings from one period in history with experimental methods from another, and to enable students to put the experience they have acquired into practice.

The situation at the end of the Pelouze episode is that students have to make decisions about the empirical formula using data from the article. In addition, they work out titration results in order to determine the molar masses of the two substances. The resulting molecular formula, $C_4H_4O_4$ for both substances, cannot be used to *distinguish* between the two different substances. Several structural formulae can be designed but not yet attributed to one of the substances.

5.3.2 The Van 't Hoff episode

The second episode is dedicated to Van 't Hoff. He published a small booklet in Utrecht, the Netherlands in 1874, on the extension in space of structural formulae:

"It becomes more and more obvious that the current constitutional formulae are unable to explain some specific cases of isomerism; this may be due to the

¹ "(...) denn unter allen Agentien scheint die Wärme hauptsächlich dasjenige zu seyn, welches die Atome vorzugsweise bestimmt, in der Anordnung veränderliche Gruppen zu bilden, worauf die Isomerie beruht." (Pelouze, 1834, p.271)

² Gewone duivekervel; Common Fumatory.

absence of a more specific statement about the real positions of atoms in space."
(Van 't Hoff, 1874, p.3)³

His proposal for the tetrahedral representation of the carbon atom "affinities" had two consequences. In the first part of the booklet, he works out a relation between the asymmetric carbon atom and optical activity (cf. Van 't Hoff, 1874, p.5). The second part is about the representation of compounds with double bonded carbon atoms (cf. Van 't Hoff, 1874, p.11). His representation of a double bond consists of two tetrahedrons connected by a common edge. Using figures of the two tetrahedrons, Van 't Hoff shows a difference in *position* between the various groups attached to two double bonded carbon atoms in relation to each other. Two different representations can be drawn up when positioning in space is taken into account.

The first example given by Van 't Hoff to show the usefulness of his new method of representation is the case of:

"(...) maleic and fumaric acids, which have defied all attempts to explain their isomerism: these acids really find themselves in the situation described above: *each of two double-bonded carbon atoms is joined to two different univalent groups, i.e. H and COOH.*" (Van 't Hoff, 1874, p.11; Van 't Hoff's italics)⁴

In a later publication Van 't Hoff gives reasons for attributing the formula with the two carboxylic groups on the same side of the double bond to maleic acid (Van 't Hoff, 1899, p.114-115). The experimental results on which these arguments are based are the formation of the anhydride, the acidic properties of maleic acid (which is stronger than fumaric acid) and of hydrogen maleate (which is weaker than the corresponding hydrogen fumarate). An explanation for this difference is given in the case of hydrogen maleate by using the electrostatic influence of a negatively charged COO⁻ on the hydrogen atom of the other carboxylic group.

The educational text includes the drawings made by Van 't Hoff to represent cases of *cis-trans* isomerism such as maleic acid and fumaric acid. Tetrahedron models can be folded by students using strips of paper. These folded structures show the rigidity of the double bond and they resemble the drawings of Van 't Hoff in that the interpretation of the meaning of the edges is also surprisingly similar to lines in the drawings (Fu-cheng He, Lu-bin Liu and Xiang-yuan Li, 1990, p.650-652).

In the educational text the decision to attribute the *cis* form to maleic acid must be made by students using Pelouze's data on the quantitative elemental analysis of maleic anhydride. Acid strength data for the substances are taken over from Van 't Hoff. These

³ "Meer en meer blijkt, dat de tegenwoordige constitutie-formules niet in staat zijn enkele isomerie gevallen te verklaren; wellicht is dit te wijten aan het ontbreken eener meer bepaalde uitspraak omtrent de werkelijke ligging der atomen." (Van 't Hoff, 1874, p.3)

⁴ "Maleïn- en Fumarzuur, ten opzichte waarvan alle verklaringen der isomerie schipbreuk hebben geleden (...): werkelijk verkeerden deze zuren in het hierboven beschreven geval: *Twee dubbel gebonden koolstof-atomen dragen elk twee onderling verschillende univalente groepen, H en COOH.*" (Van 't Hoff, 1874, p.11; Van 't Hoff's italics)

data have to be combined with the results of the titration experiments carried out by the students in the first episode.

At the end of the second episode, it should be clear which structural formula belongs to which substance. The structural formula can already be used for explaining properties of the substances. Students can also use their knowledge of the nomenclature to give the systematic names. However, no arguments are offered in the text for the decision to reject the structural formula of the nonexistent substance 1,1-butenedioic acid.

5.3.3 *The Lewis episode*

The third episode focuses on the book "Valence and the Structure of Atoms and Molecules" (Lewis, 1923).

Lewis mentions maleic acid and fumaric acids when he wants to put into practice a theory on the prediction of properties. The theory predicts that maleic acid and fumaric acids are equally strong acids because the distance, in terms of numbers of carbon atoms, between both carboxylic groups in the structural formula is the same:

"Here the number of atoms separating the two carboxyl groups is the same in both acids, and we might therefore expect that the dissociation constants would be very nearly the same." (Lewis, 1923, p.144)

He knows, however, that this is not the case, and remarks:

"It seems evident that there is an opportunity for spatial approach of the two carboxyls in the one case which is absent in the other, and that this approach enormously heightens the mutual influence of the two groups." (Lewis, 1923, p.144)

This uncertainty of the applicability of the theory in relation to the structural formulae is remarkable, in view of the explanations of Van 't Hoff mentioned above. It is even more remarkable because current explanations for the difference in acid properties are based on the occurrence of hydrogen bonds. Lewis himself proposes "the suggestion of what has become known as the hydrogen bond". He regards this as "the most important addition to my theory of valence" (Lewis, 1923, p.109). The suggestion of a hydrogen bond is that "an atom of hydrogen may at times be attached to two electron pairs of two different atoms, thus acting as a loose bond between these atoms." And in the case of two water molecules: "The atom of hydrogen attached to the two oxygen atoms represents the new type of bond" (Lewis, 1923, p. 109-110). But Lewis did not use the hydrogen bond to explain "the mutual influence of the two groups" (i.e. the "two carboxyls").

This information about the two substances is incorporated in the educational text. Use is also made of the theoretical notions Lewis developed, such as his model of the structure of the atom, the group of eight (called 'octet' by Langmuir) and electron pairs:

"The electron pair, especially when it is held conjointly by two atoms, and thus constitutes the chemical bond, is the essential element in chemical structure."
(Lewis, 1923, p.97)

Lewis' advice to observe the limitations of the various rules, including the octet rule, is also mentioned in the educational text.

In the third episode, the meaning of the dash in the structural formulae is extended to that of an electron pair. An opportunity is offered to use the structural formula to explain the difference in acidic properties of the substances, based on the assumption of hydrogen bonds. It might be conflicting that Lewis's view (of a hydrogen atom as a bonding atom) does not fit in with what students have learnt in earlier years at school (hydrogen bond as an electrostatic effect between areas of partial positive and partial negative charges). This conflict, if it arises, requires decision-making by students on the applicability of earlier acquired knowledge.

5.3.4 The Yardley episode

Crystallography is introduced in the fourth episode, not only so that students can understand Yardley's publication at the centre of this episode, but also because the techniques and methods of investigating crystals are considered relevant for modern chemistry education. Furthermore, it offers students an opportunity to look at solids and interactions *between* molecules. Up to now, the molecule's environment has not been taken into account.

Yardley (Lonsdale-Yardley) reports on her work at the Davy-Faraday laboratory in London in an article entitled "An X-Ray Examination Of Maleic and Fumaric Acids" (Yardley, 1925).

She investigates crystals and is especially interested in a question about symmetry of molecules in crystals:

"The following investigation was undertaken primarily to determine whether the planosymmetry and centrosymmetry usually ascribed to maleic and fumaric acids respectively have any actual existence in the crystalline state." (Yardley, 1925, p.2207)

According to Meyer and Jacobson (1907, p.800) plano- and centrosymmetry mean respectively *cis* and *trans* in the molecule, and they consider that the older terms should not be used any more, at least not in organic chemistry.

In the educational text, the two terms, plano- and centrosymmetry, are used for an assignment on the symmetries which can be found in the *cis* isomer and in the *trans* isomer. Yardley's investigations offer the information to students to explain the relatively high melting point and moderate solubility of fumaric acid as compared with maleic acid, with "a closer association between the chemical molecules than that usually existing in crystals" (Yardley, 1925, p.2217).

Because crystallography is new for students, other publications are used to give appropriate background information (Escher, 1935) and to provide a link with relatively recent experimental results. Information on angles and distances in molecules and about electron density differences is not derived from a single publication by one person, but is drawn from publications by a number of 'crystallographers'.

In the Yardley episode, the crystallographic data and electron density plots enable students to question the length and the assumed reactivity of a double bond in systems thought to be conjugated. The experiment with maleic acid and bromine in light is intended to stimulate a discussion on the various meanings of the two dashes of the double bond in reaction with bromine.

5.3.5 The fifth episode and the global context

The fifth episode differs from the four others. No specific publication or person has a central place in the last episode, for two reasons. First, as so many people are working with both substances it seemed impossible to select one. Secondly, the idea was to shift the focus to the students themselves. They might recognize the two substances in applications in daily life as food additives or medicine. Furthermore, the knowledge of chemistry they have already built up could be brought in here. Aspects of the structure-property relations can be found in the school chemistry of polymerization reactions and of stereochemistry.

The educational text invites the students to work on assignments on these structure-property relations. An experiment is included which elaborates on earlier experiments with bromine and with isomerization. This is a version of an experiment on a reaction mechanism for the isomerization of maleic acid to fumaric acid by Meek (1975, p.541-543). Students are asked to propose a possible reaction mechanism that can also explain the results of experiments in earlier episodes. In this experiment, the structural formula is used to describe a process, i.e. a new layer of meaning is added. As no answer is proposed by Meek, this is an open-ended experiment to both teachers and researchers. As such, it seemed an appropriate final assignment about gathering knowledge in a decision-making process.

The episodes of the narrative were designed in the light of results from earlier chemical research, as published in scientific journals and books. This was meant to let students work in an explorative way. The students had to interpret the information offered, verify the information, mobilize their knowledge acquired earlier, make decisions as they work towards establishing the structural formulae and various meanings of these formulae.

Students should reach consensus in discussions on the assignments and communicate their decisions on structure-property relations in structural formulae in a way that is meaningful for themselves and acceptable to the teacher.

I relate the necessity for making decisions and other activities mentioned above to creating knowledge as a human endeavour and I see this creation of knowledge as the global context of the educational text 'Kennis Maken'.

5.4 The Assignments in the Educational Text

In the two preceding sections I discussed the chemistry content and the narrative format of the educational text 'Kennis Maken'. The educational text as a whole might be regarded as a hypothesis in the educational experiment as to what is expected from the students. However, parts of the text, i.e. the assignments, are more accessible for investigation than the whole text. Therefore, I focus on the special role of assignments in the text with regard to the educational experiment. The results expected from a number of assignments are discussed (5.4.1) and actual results of these assignments when the text was trialled in the classroom are presented (5.4.2). The titration assignment appeared to be a special case during the preliminary trials and also during the educational experiment in the classroom. Therefore, this assignment and its experimental results will be discussed in detail in the following sections (5.5 and 5.6).

5.4.1 The purpose of the assignments

Assignments are a valuable part of any educational text, experimental or not. The function of assignments in general might be described as supporting the sequence of concepts. Assignments designed for this purpose are included in a text with a view to extending a meaning or practising with a newly-learned concept.

In the educational text of 'Kennis Maken', the function of assignments can be described as: *creating the opportunity for a dialogue with the text*. This means that students, while working with the text, find their own way around the body of information offered and are drawn into activities by means of the assignments.

I regard the dialogue function of the assignments as valuable both *for education*, because it enables students and teachers to communicate on the tasks at issue, and *for educational research*, because it allows the researcher to obtain research material by listening to discussions, observing activities or reading the reports of the assignments.

In Section 5.1 I mentioned three criteria for designing the educational text, i.e. guiding principle, sequential contingency and global context. Each of these can be associated with a dialogue function of the assignments. The assignments which deal primarily with the substance and their properties fit in with the guiding principle of starting from the substance itself and therefore open the way to a *dialogue with matter*. Verification assignments which usually follow the sequential contingency of the molecular structure theory lead to a *dialogue with the text*, either the written information or the information given in the quotations. The dialogue function developed in the 'open' assignments can

be regarded as belonging to the global context of communication between people i.e. a *dialogue with each other*. It will be noticed that in all assignments, these dialogue functions are present. However, some assignments focus more on the properties of the substances than others, and 'open' assignments offer more opportunities for discussion than verification assignments.

I give some examples of these three kinds of assignments because I use this classification to describe the results of the educational experiment: 1. assignment with substance, 2. verification assignments and 3. 'open' assignments.

ad 1. The first assignment in the educational text is about observing the formation of white crystals halfway up a test tube. The experiment is an adaptation of the experiment by Pelouze (1834, p.265). A demonstration is carried out by heating malic acid in a test tube in a thermostated oil bath kept at 190°C. As oil baths are usually not found in school laboratories, the use of a domestic deep-fryer was advised. In the subsequent assignments, students are asked to experiment with the newly formed substance. However, the amount of the white substance formed in the oil bath experiment is not enough for all groups to work with. Therefore the school supply must be used. The aim in the assignments is to induce the students to set up a chain of thought with the substance as starting point.

ad 2. Verification assignments are to check, either by experiment or by argumentation, whether results obtained by others are reliable, and whether the claims are valid. The second experiment in the text for verifying the properties of solubility, acidity and precipitation reaction, is intended to draw the attention of the students to the properties of the substance. This should enable them to see similarities with and differences between other substances. They are invited to look for other properties apart from those mentioned by Pelouze (after consulting the teacher). The students should use the knowledge they already have, and they should decide if they agree on the information provided.

ad 3. The 'open' assignments are either on assessing the results of experiments or the interpretation of data from the literature. 'Open' means that students, for instance, have to select the relevant information from tables containing fairly ambiguous data. An example is the assignment to calculate the mass ratio for the empirical formula with the experimental data from Pelouze's article (Pelouze, 1834).

	I.	II.	III.
Kohlenstoff	41,30	41,32	41,31
Wasserstoff	3,46	3,44	3,60
Sauerstoff	55,24	55,24	55,00

Diese Analysen führen zu folgender theor. Zusammensetzung:

1 At. C =	76,438	41,84
1 — H =	6,239	3,41
1 — O =	100,00	54,75
	182,677	100

Figure 5.1 Data from Pelouze's article (1834)

Students have to decide whether to use data from one column only, or to use a mean value. The decision-making process is expected to lead to discussions.

Another example of an 'open' assignment where there is no foregone conclusion is when the experiments carried out by the students themselves yield different and perhaps conflicting results. The titration experiments provide this 'openness'. Then a consensus must be reached in the group on which values should be used and how to interpret these values.

If an educational text is designed for an educational experiment it might be expected that specific assignments have to be included for the purpose of stimulating discussions and activities, and therefore for the researcher to be able to collect more research material. In the case of 'Kennis Maken', the dialogue function appeared to be productive enough for that purpose and no assignments were designed specifically for educational research purposes.

Valuable research material was obtained, for two reasons.

Firstly, the method of working in small groups of three or four students was preferred for the educational experiment. Students have to reach a consensus on common answers to the assignments, and therefore they have to discuss the 'work in hand' with each other. Talking to each other and trying to reach a consensus fits into the global context of people creating knowledge. Furthermore, talking with each other yields research material if these discussions are recorded on tape.

Secondly, the 'open' assignments offered opportunities for various different interpretations and therefore required the same kind of group discussion to reach a consensus. Discussing and defending interpretations to work out a consensus fits into the global context. At the same time, working with 'open' assignments, especially when opinions and the level of comprehension differ, yields research material in written or spoken form.

The educational experiment was conducted under the following circumstances.

Two teachers at two schools expressed their willingness to use the text in their classes as additional material for revision and extension of the subject matter. The period in which the educational experiments could take place was just before the last assessments, prior to the final examination. This meant that the students had already covered all subjects mentioned in the prescribed exam syllabus (Eindexamen-programma, 1984).

The teachers consented to my presence during the lessons. This gave me the opportunity to observe. Sometimes I got involved as participant in the lessons through questions asked by students, and more explicitly in the role of the author of the text who therefore was supposed to know all the answers. That was the reason why I occasionally took up the role of a teacher. This might be regarded as a drawback from the point of view of the researcher, because I provided answers to students' questions. On the other

hand, the advantage of my earlier experience as teacher made it possible to link students' comments to subject matter taught in previous years.

As mentioned above, students worked in small groups of three or four, independently of the teacher for most of the time. Occasionally, the teacher called all the groups together in order to bring forward some points related to concepts taught earlier. The time reserved for the educational experiments was eleven fifty-minutes lessons in both schools. Some group discussions were recorded on tape and transcripts were made of some parts of the recordings. Also, written group answers and reports became available. Permission to use the anonymized material for research purposes was granted by students and teachers.

5.4.2 Observation report on the assignments

In the following I examine the results of the assignments in the educational experiment on the basis of my observation notes. I deal with them in the same order: first the assignments on a substance, followed by the verification assignments and then the 'open' assignments.

The results of the first assignment were rather disappointing: in one school the experiment could not be carried out. In the other school it appeared that the use of a deep fryer did not allow all students to have a good look at what was going on in the test tube. The aim of achieving a chain of thought based on the substance was not fulfilled in the first assignment of 'Kennis Maken' in the sense that students were not involved and did not comment on the white crystals formed in the first experiment in the biography. With hindsight, some reasons for this should have been evident. No time was reserved in the educational text to observe the substance in more detail, to describe the shape of the crystals, for instance. The experiment was not carried out by the students themselves. Seeing a substance formed in one's own experiment is not the same as seeing it formed from a distance in an experiment carried out by someone else (cf. De Vos and Verdonk, 1985b). Furthermore, a substance seems more special when one has made it oneself, rather than just being issued with school stock. One group was not in favour of the assignment because in their opinion, carrying out an experiment to demonstrate the formation of a substance is a waste of time: "why do something you know already".

Students regarded the assignment in which the results of Pelouze had to be verified as suitable for school practice. They found that the substance was soluble and the solution turned red with litmus. However, the results indicated that besides verifying someone else's statements, the assignment also verified the students' own knowledge. The students were asked to use their existing knowledge, and apply it in another situation. This proved to be more difficult than intended. Students know that lime water is a reagent for carbon dioxide. When lime water was added to the dissolved substance, some students remarked: "no precipitation, no carbon dioxide present". Presumably they did not consider the possibility that the calcium salt of the substance could precipitate.

Verification assignments, such as "Examine whether this statement is true", are common in school practice. Several groups paid a lot of attention to the verification assignments. Some lively remarks were passed, such as "the man might have" while commenting on the results of Pelouze. It seems that students can talk more easily about the problems they encounter when these problems are someone else's. I see this as an example of a dialogue with the text.

The 'open' assignments can be regarded as successful from the point of view of educational research. In the assignment on the mass percentages, the students found choosing between the columns of data an interesting experience. They discussed, sometimes lengthily, their preference for taking data from one column or for using an average of the three columns. However, the calculations turned out to be rather difficult. Some groups did not see the link with corresponding problems they must have encountered before. It was remarkable that different groups performed the calculations in a different order. In some cases, the order in which calculations were performed led eventually, after some discussion, to a 'correct' answer in the intended chemical sense of a mass ratio $C : H : O = 1 : 1 : 1$ for the empirical formula $(CHO)_n$.

From the educational experiment it can be concluded that in 'open' assignments, calculation sequences should be taken more into account. This was clearly the case in the 'open' assignment with the titration experiments. I will discuss the titration assignment in detail in the following section.

5.5 The Titration Assignment

The titration experiment is an assignment in the first episode of 'Kennis Maken'. In the introduction to the assignment the objective is discussed: a molar mass of the substances under investigation must be known in order to decide on a value for n in the empirical formula $(CHO)_n$. The students know that the substances are acids but they are not aware that the acids are bivalent. Therefore, the choice of two indicators is prescribed, i.e. methyl orange and phenolphthalein. The assignment is as follows:

Experiment 4 *Titration of solutions with sodium hydroxide solution*

In order to obtain as much information as possible, four titrations are carried out at the same time: two with moss acid with two different indicators, and two with the Pelouze's acid with the same two indicators.

Weigh approximately 200 mg acid.

For dissolving moss acid, add 5 ml ethanol.

Add 10 ml distilled water.

Add 5 drops of indicator solution.

Titrate with 0.10 M sodium hydroxide solution until the indicator changes colour.

Calculate for each titration how many mol H^+ reacted.

Collate the results of all groups and try to decide on a molecular formula.

Students are well-acquainted with the experimental procedure of an acid-base titration, but they have to apply it in a different way here. The titration results are not to be used, as common in school practice, to calculate the concentration of a solution. In the educational experiment, students should use the results to calculate a molar mass, to decide on a possible value for n and subsequently to give various representations in the form of structural formulae. From the preliminary trials of the titration during and after writing the educational text it became clear that using the titration in another way called for a closer look at the special features of this particular titration (5.5.1). I examine the order in which calculations with the titration results might be performed (5.5.2). Subsequently, I discuss the consequences of carrying out the titration using a pH meter and I refer to the experiences of a group of students during the educational experiment in a classroom (5.5.3).

5.5.1 Mobilizing prior knowledge

The idea of using a titration experiment to calculate the molar mass was inspired by assignments from older chemistry books (cf. Van Meurs and Baudet, 1957, p.169). This titration experiment is part of the titration tradition of quantitative analysis.

Although not belonging to the current school practice, the experiment might be known by students; at least it was by Mo in the following fragment:

- Be No, I'm titrating. Titrating is what it says here
 G And, why
 Be Well, using acid
 Mo I thought determining pH, but I do not know if that's any use. You can the molari, what is it called
 La You name it (?)
 Mo You can determine the number of grams, the weight which you have dissolved, and if you're titrating then you can determine, well how do you do that.
 You dissolve the solid matter, you titrate with sodium hydroxide solution, I suppose, then you can determine how many moles it is. The weight
 Be Use the definition
 Mo Determine the molar mass of that $C_nH_nO_n$.

Prior to the titration experiment, the students know that there are two white substances and they verified several properties, establishing for example that the substances were acids and simple organic compounds. The empirical formula is known and written as $(CHO)_n$ or as the element ratio of 1 : 1 : 1. In general, if the value of the molar mass or of the molecular mass is known, the value of n in the empirical formula can be established.

In the school context, several assumptions with regard to 'simple' organic compounds are implicit:

- there are no other elements than C, H and O;

- n is an integer and even⁵;
- n is as low as possible;
- the acidic properties of the organic acids are only attributed to carboxylic groups and each titration step corresponds to one acid group.

The titration is an acid-base type which students have carried out several times. In the usual procedure, an acidic solution of unknown molarity is titrated with a solution of hydroxide of known molarity. When the acid is neutralized by the hydroxyde, the end point of the titration is visible by the change of colour of an indicator, or by a steep slope in the titration curve when the titration is monitored by a pH meter. The molarity of the acidic solution can be calculated provided the basicity of the acid is known.

So far, the titration can be expected to follow its normal course. However, the following points may cause difficulties because they deviate from this procedure.

- It is not a precisely measured volume of the acidic solution that is used for the titration. First, an amount of the substance is weighed accurately, and then dissolved in a (small) but not precisely known volume of water. This solution is titrated.

- The two substances, Pelouze's acid and moss acid, are bivalent acids, but the students are not aware of this. Knowing the bivalency is essential for the calculation of the value of n . The titration results have to show two equivalence points. Therefore, the instruction is to carry out the titrations using two indicators. The first is phenolphthalein (range: pH 8.2, colourless - pH 10.0, purple), as could be expected for the titration of a weak acid with a strong base. The second is methyl orange (range: pH 3.1, red - pH 4.4, orange yellow), which can indicate an end point if the acid being titrated is strong enough, as is the case with the Pelouze's acid, i.e. maleic acid. However, when moss acid which is a weaker acid is titrated with methyl orange as indicator, the colour changes so gradually that results of various titrations will show a range of titration values. Titration results, i.e. how much of the hydroxide solution (ml) was used for changing the colour of the indicators methyl orange and phenolphthalein respectively, can be presented as:

Pelouze's acid:	17 ml	34 ml
Moss acid:	(13 ml)	34 ml

- The titration values are not presented in the 'normal' way for titration results: it is customary to give the value to one or preferably two decimals when a 'normal' 50 ml burette is used. It is not necessary to be more precise in this case however, because the value of n is an integer. The value of 13 for the first equivalence point of moss acid is a value decided upon by students in one of the classroom titrations. The values of 17 and 34 are theoretical but were also found regularly during the experiments.

These values are used in the following discussion on the calculations.

⁵ n must be even, since each bond requires two valencies and the total number of valencies in CHO is 7.

5.5.2 Calculation sequences

The titration experiments were tried out in the classroom but also discussed in groups of chemistry teachers and educators at workshops and pre- and in-service courses. It emerged from the discussions in these trials that various sequences are possible for the calculation of values for n . In order to compare two calculation sequences I work out these sequences, making them look as unlike as possible by accentuating the differences. One I recognized from my teaching experience as belonging to the acid-base titration context of the school practice, the other one I could not recognize at first.

200 mg acid, empirical formula $(\text{CHO})_n$, was used.

When the indicator, methyl orange, changes colour 17 ml 0.10 M hydroxide solution has been added.

That means $17 \text{ ml} \times 0.10 \text{ M} = 1.7 \text{ mmol OH}^-$ has reacted.

There was 1.7 mmol H^+ . Therefore, assuming the acid to be monovalent in this titration, there was 1.7 mmol acid.

1.7 mmol acid corresponds to 200 mg acid.

Suppose the molecular mass of the acid is $M \text{ g}\cdot\text{mol}^{-1}$

Then $200 \text{ mg} : M \text{ g}\cdot\text{mol}^{-1} = 1.7 \text{ mmol}$

This gives for the value of $M = 200 : 1.7 = 117.6$

By using the empirical formula $(\text{CHO})_n$, the value of the molecular mass can be expressed as $M = (12 + 1 + 16) n = 29 n$

Together, this gives $29 n = 117.6$ and therefore $n = 117.6 : 29$,
and thus $n = 4.1$

n must be an integer, therefore $n = 4$.

The molecular formula is then $\text{C}_4\text{H}_4\text{O}_4$.

The other calculation sequence is:

200 mg acid, empirical formula $(\text{CHO})_n$, was used.

$1/(12+1+16) = 1/29$ part of the mass is hydrogen.

200 mg acid contains $1/29 \times 200 \text{ mg} = 6.9 \text{ mg}$ hydrogen.

When the indicator, methyl orange, changes colour 17 ml 0.10 M hydroxide solution has been added. This corresponds to 1.7 mmol of the base.

From the total amount of hydrogen available 1.7 mmol is used for the neutralization reaction: 1.7 mmol or 1.7 mg of the hydrogen available reacted as acid.

Of the total amount of hydrogen available $1.7 \text{ mg} : 6.9 \text{ mg} = 0.25$

or $1/4$ part reacted as acid.

This means that the lowest possible value of n for hydrogen is $n=4$.

The same applies for carbon and oxygen.

The molecular formula is then $\text{C}_4\text{H}_4\text{O}_4$.

When these two calculation sequences are carried out with the results of the titration of the Pelouze's acid with the indicator phenolphthalein, the amount of hydroxide

solution used is 34 ml. The first calculation sequence then gives that $58.8 : 29 = 2.0$, and thus $n = 2$.

The answer to the second sequence is $3.4 : 6.9 = 0.49$, or $1/2$ part of the available amount of hydrogen is acid. If the notation $1/2$ is used the conclusion will be that $n = 2$. However, if the notation is rewritten as $2/4$, it might be 4. Of course, this interpretation is only possible when there is a notion of the acid being bivalent.

Both calculations show a different calculating sequence but both sequences are meaningful in the chemistry context.

It so happened that some students used a third method to decide on the values of n , this time by using their knowledge of structural formulae and the valencies of carbon (4), oxygen (2) and hydrogen (1). Knowing about simple organic substances, students looked for structural formulae with the lowest possible value of n . Furthermore, knowing that these substances are organic acids is a help, because students know that organic acids contain the COOH group in which H represents the acid nature of these substances.

Once they had found the empirical formula $(\text{CHO})_n$ most students started to talk about possible structural formulae, sometimes expressing their amazement at the unusual ratio of C, H and O being 1 : 1 : 1. Drawing possible structural formulae leads to the rejection of the value $n = 2$, because no proper formulae can be drawn.

From the above-mentioned analysis, it appears that various sequences of calculation and reasoning are possible for handling the titration results. In the following I go into the consequences when the titration is performed by using a pH meter to monitor the course of the reaction.

5.5.3 Consequences of using a pH meter

The openness of assignments allowed the students to take initiatives.

A group of students decided to monitor the course of the titration reactions by means of a pH meter in addition to a titration with the indicator.

- Be I think it is better to do with several indicators.
La You can do both, can't you.
Mo I think the pH curve is not a bad idea
Mo pH curve where the point lies
Be And you can see if it is a bivalent acid at the same time
Mo And you can see if it is bivalent acid at the same time.
That really is an advantage.

The results of the first round of titrations were the following: students started with the titration of the Pelouze's acid (maleic acid) with phenolphthalein. They found 34 ml of sodium hydroxide solution and then they calculated that $n = 2$. The titration with the pH meter carried out at the same time gave two equivalence points, and therefore they came to the conclusion that the Pelouze's acid had to be a bivalent acid.

- La Found two points
Perhaps a third one
- Mo With your data that it was a bivalent acid and the data we found from the titration I've worked out $n = 4$.

Having decided on $n = 4$, they proposed to draw two structural formulae, i.e. of a 1,2-butenedioic acid and of 1,1-butenedioic acid.

But then the titration with moss acid (fumaric acid) was carried out. This titration has first of all the complication that the acid does not dissolve easily. The main problem turned out to be that the titration results with the pH meter *did not show two end points*, that *34 ml was needed* for the titration and that therefore the *value of $n = 2$* had to be decided upon. These results unsettled everything they had found in the earlier experiments. They became confused and could not find a satisfying explanation for their own experimental data.

- Mo Monovalent acid
Be Must be
(...)
- Mo Listen, if, if you figure it out, the whatsit. If you work it out with the value you just determined then you find $n = 2$. That can't be right.
- Dr What d'you mean, it can't be right
- Mo Then moss acid should have the formula of C_n , eh, $C_2H_2O_2$.
- Dr So what?
- Mo Try to make a monovalent acid and an acid from O, O, H, C, and you've got one H left.
- Dr Hard luck, I can't help it
- Mo Moss acid with fff (*phenolphthalein*) is no good, Then we have to use methyl orange. Then we can (...) has an end point, a lower pH, where is its end point.

The students used figures from a table on the blackboard listing the results of the experiments of all groups in order to have experimental information gained by using methyl orange. However, they then encountered another problem, i.e., the available results of the titration experiments of moss acid using methyl orange as indicator consisted of the values 11.9 and 13.0. The calculation carried out with these values did not help to overcome their confusion. The titration experiments which were at first so successful, ended rather unsatisfactorily for them. Their own initiative to use the pH meter had not made things easier for them. If their knowledge of chemistry at that time had allowed them to interpret the titration curves of weak acids, they might have come to the conclusion that the acids are bivalent. However, this is not normally part of the school programme.

During the educational experiment, the students did eventually arrive at the intended result, *viz.* deciding together on a value of n while discussing possible structural formulae. However, they were not satisfied because they could not interpret their own experimental results and they could not find an answer to the difficulties themselves. Furthermore, the discussions took much more time than was expected. The classroom experiences reported above showed that the titration assignment should not be as open as intended in the first design. The number of implicit assumptions may have been too large, especially with regard to the acid being bivalent, because this knowledge is crucial in deciding on the values of the titration data of fumaric acid. A result with consequences for further educational analysis is that a closer look is needed into the differences between a titration with indicators and one using a pH meter.

I interpret these two ways of carrying out the titration experiments as using different contexts. The experiences with the calculation sequences can also be interpreted as a difference of context. This is to be discussed in the next section.

In this subsection I discussed the titration assignment using the experiences of a group of students working on the assignment. One might wonder how a group of students could really become so involved in an assignment that caused so many troubles. It might look like having 'ideal' students for the educational experiment rather than 'average' students. The group working with titration curves was indeed absorbed by the titration experiments, but they turned out to be quite normal by skipping other assignments because of lack of time or interest. They copied the results of other groups. (This was acceptable because division of labour can be regarded as part of normal scientific practice.) They did not do the folding assignment. However, I conclude from the attention and time spent on it during the discussions in the class, that they were intensively involved with the titration problems. They had to handle uncertainties and make decisions. In discussing their own conclusions they were active in the process of creating knowledge.

5.6 Titration, Correspondence Terms and Sequence of Contexts

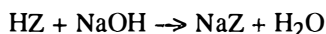
In this section I compare the two titration procedures I reported in the previous section with the methods of calculating and deciding upon a value of n (5.6.1). I link the procedures and the calculation sequences to various contexts described in the correspondence terms worked out in Chapter 3. Next, I give a tentative educational structure for molecular chemical bonding. This is the basis on which the educational text is adapted for the next cycle in the educational experiment (5.6.2).

5.6.1 Titration in different contexts

The two ways of carrying out the acid-base titration experiment are a titration with two indicators and a titration with the pH meter. These two methods have different characteristics which I compare with each other and, subsequently, with the calculation sequences.

1. Titration with indicators belongs to an analytical chemical context. The usual objective for an acid-base titration is to determine the unknown amount of an acid (a base) with the known amount of a base (an acid). A sudden change in colour of the indicator shows the equivalence point of the titration.

The reaction can be expressed as:

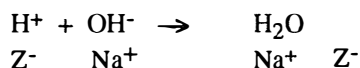


The stoichiometry of the neutralization reaction which is supposed to proceed to completion is shown in this way. Balancing the equation implies counting the elements. Elements can be regarded (and even defined) in terms of 'mass portions', or in terms of atoms, depending on which point of view is taken, the phenomenological or the corpuscular. In both cases, the objective of the titration is to determine the amount of hydrogen available for the neutralization reaction, and this amount is expressed in mass units or in moles.

I connect the second calculation sequence (cf. 5.5.2) with this conception of the titration, because there the amount of hydrogen which reacted is calculated in *mass* units.

2. Titration by means of the pH meter belongs to a physico-chemical context. During the titration the change of the concentration of H^+ ions is measured as a result of adding a known amount of a base (acid) solution. Plotting the successive pH values in a diagram show the course of the reaction. A steeply rising or falling slope is associated with a relatively sudden change of the pH value around the equivalence point. This can be used to determine when equivalent amounts of H^+ and OH^- have been present. However, more information can be obtained from the shape of the graphs before and after the steep section. These graphs can be interpreted in terms of the strength of the acid (base) and in this way, they represent the reactivity of the acid (base).

The notation of the equation appropriate for the above view of the titration is:



Balancing this equation is performed by counting atoms and *charges*. The calculation sequence mentioned first in Section 5.5.2 seems to be appropriate for this titration procedure because H^+ and OH^- are also mentioned there, although the assignment in the educational text did not require the use of the pH meter.

I emphasized the differences between the above-mentioned methods of titration for the purposes of analyzing the results of the educational experiment as well as the

chemical experiments. In this sense, I am continuing the educational analysis. In school practice, the notation of the equation in ions and the first calculation sequence are commonly used. This also applies to titrations using indicators and assignments in the analytical-chemical context, and not only to titrations using a pH meter.

3. The third possibility I mentioned of deciding on the value of n in the titration experiment is by taking into account the supposed position of an acidic H in the first calculation sequence (cf. Section 5.5.2). The process of deciding on the basis of the results of the titration starts from the other end, i.e. structural formulae with carboxylic groups (COOH) that are possible with the empirical formula $(\text{CHO})_n$. The question is then: how many Hs are in a special *position* in each structural formula representing the property of acidity. Or, in other words, how many Hs might split off and react in an acid-base reaction.

The notation of the equation might be the same as what results from the first calculation sequence, but prior to this notation, structural formulae will be sketched with help of (co)valence rules. Equations should be balanced by comparing structural formulae. What might be counted is probably the number of carboxylic groups, or the number of Hs in a special position.

The three descriptions of the titration assignment in the educational experiment are summarized as follows:

Mass amount hydrogen	counting mass	substance-based
Amount of hydrogen ions	counting charge	ion-based
Hydrogen in 'acid' position	counting 'dashes'	structure-based

In the next subsection I use the interpretations of the titration procedures and calculations mentioned above. I relate the titration descriptions to various contexts and look for another point of view on how to adapt the educational text for the second round in the educational experiment.

5.6.2 Contexts in the episodes and contexts in an educational structure

In the table given above, I distinguish three different contexts: *mass* context, *charge* context and *structure* or *distance* context, to use a term I introduced earlier. *The titration assignment can be considered from the point of view of each of these contexts.*

Distinction between contexts has been dealt with in previous chapters. Here is a short summary. In Chapter 1, I described the sequence of atomic structure followed by chemical bonding as a transition from an energy context to a distance context. In Chapter 3, I pointed to a difference between the energy context of the free atom and the distance context of the bonded atom, which I called the Lewis atom. The sequence of going from a free atom to an atom bonded in a molecule can be described as going from an energy context to a distance context.

In Section 4.3, I elaborated on the correspondence between the macroscopic world of substances and the microscopic world of the corpuscular models as a continuation of the model characteristics of Chapter 3. I described the relation in correspondence terms: mass, distance, charge, time and energy.

I will now use the attribution of these correspondence terms to the various contexts to describe the titration assignment.

The objective in the educational text is to work from the composition of a substance towards a structural representation. The titration experiment has a central role in the transition from the empirical and molecular formula to the structural formula, representing both substance properties and molecular structure. This can be described in terms of transition between contexts.

The distinction between the two substances maleic acid and fumaric acid cannot be represented by means of the empirical formula $(\text{CHO})_n$ calculated *from mass measurements in the mass context*. Nor can the distinction be represented by the molecular formula $(\text{C}_4\text{H}_4\text{O}_4)$, therefore when the value of n is available if the calculations are performed within the mass context. The distinction can be expressed only when there is a possibility of representing of atoms in a specific *position* in relation to each other: *a structural formula in a distance context*.

Therefore, the transition from the molecular formula to the structural formula can be described as going from the mass context to the distance context.

As a result of the titration difficulties in the educational experiment, I recognize the possibility of different contexts being present and subsequently I interpret the transition from an empirical and molecular formula to a structural formula as a transition from a mass context to a distance context. For the educational experiment, this means that in addition to the interpretations of structural formulae, it is necessary to see how students use the various contexts and their differences and how they handle the transition from one context to another. *A tool for recognizing the relativeness of models and structural formulae might be found in the comparison of the contexts of the molecular and the structural formula*. However, because the group of students mentioned above was mainly preoccupied with deciding on the value of n , while they used sketches of structural formula (cf. the third calculation sequence in Section 5.5.2), it was difficult to expect a comparison of the contexts.

With regard to the contexts of time and energy, these are not dealt with explicitly in the educational text. Attention focuses primarily on substances, i.e. states of matter and, only in relation to them, reaction properties. Therefore the time context is not taken into account and no reaction kinetic properties are included in the text. With regard to the energy context, the educational text is not designed by starting from an energy context. This is connected with the results I reported on in the first two chapters of this thesis.

In Section 5.2 I remarked that representing various reaction possibilities in the dashes of the structural formulae might have consequences for the meaning of the element symbols in the structural formulae.

I will now summarize a sequence of meanings of the dashes and of the element symbols in the subsequent episodes by linking these to the sequence in contexts as described for the development of the formulae.

In the Pelouze episode the symbols refer to atoms, meaning 'mass portions' of elements (relative, not absolute). The dashes refer to bonds meaning '*belonging together*' (association). The context which predominates in the Pelouze episode is the mass context.

In the Van 't Hoff episode the symbols refer to small objects in space (sphere, tetrahedron, cube). The meaning of a dash is '*the closest distance in space*' (neighbourhood). The context which predominates in the Van 't Hoff episode is the distance context.

In the Lewis episode the symbols refer to an atom meaning 'kernel' (nucleus without outer electrons). The dashes refer to bonds meaning '*shared electron pair*' (attraction). The context which predominates in the Lewis episode is the charge context.

In the educational text 'Kennis Maken' the mass context, the distance context and the charge context feature in that order. However, when the transition from one episode to another is made, the meaning of the dashes and the element symbols in one episode will be maintained in the subsequent episode.

In the Pelouze episode the mass context dominates, for instance, by representing the composition in symbols and in empirical and molecular formulae.

The Van 't Hoff episode is characterized by the distance context when the difference between the twin pair maleic acid and fumaric acid can be expressed by differences in position in structural formulae and corpuscular models. But the mass context is still present, i.e. the structural formulae are to be considered in a mass + distance context.

In the charge context of the Lewis and Yardley episodes, mentioning electrons is not followed by a change in the structural formula depiction with regard to the covalent bond. However, layers of meaning are added not only because reaction possibilities have to be represented, but also because in the charge context, both previous contexts are present. Once the meaning of electron pair is added to the meanings of a dash, the structural formulae are to be considered in a mass + distance + charge context. Furthermore, the introduction of the hydrogen bond in the Lewis episode has a consequence for the pictographic form of the structural formulae, i.e. a dotted line depicts the hydrogen bond.

In the description given above, I indicate a tentative educational structure.

The tentative educational structure of molecular chemical bonding is formed by the successive steps in the development of the structural formulae in relation to the sequence of the mass context, mass + distance context and mass + distance + charge context.

In the educational text, the concepts within contexts and the way the contexts succeed each other should be presented in a coherent way. By taking into account the sequence of contexts, mass, distance and charge, the sequential contingency of the recontextualization can be improved.

Trying out the educational text in an educational experiment may lead to conclusions on the design of the text. The guidelines for recontextualization were formulated as guiding principle, sequential contingency and a global context. The use of the text in the classroom might give an answer as to whether these guidelines are useful for designing an educational text in the framework of the educational development.

I will discuss the consequences for the adaptation of the educational text for the second round of the cyclic procedure in the next chapter.

In the framework of this thesis, the educational text is to be regarded as an instrument for answering questions from the research project on chemical bonding. The issue for the concept developmental research part of the research project is whether, by using the text, students will gain more insight into working with models in the chemistry context.

6 Creating Knowledge in an Educational Experiment

In the framework of the research project on chemical bonding, I revised the educational text 'Kenniss Maken' as part of the cyclic procedure of research and development (cf. Section 4.1). On the basis of results of the first educational experiment, alterations were incorporated in order to advance the objectives of the educational text. The educational text was written for the educational experiment to investigate, among other things, teaching the idea of relativeness of models in the chemistry context. I used three recontextualization guidelines to describe the design of the educational text: the global context, the sequential contingency and the guiding principle. These guidelines were applied in 'Kenniss Maken' in, respectively, creating knowledge as a human endeavour, the molecular structure theory, and starting from the substance.

Section 6.1 describes some of the adjustments, referring to the guidelines for recontextualization and the results of the first experiment. In Section 6.2, I report on the choices and decisions behind designing and writing the closing episode in the revised version. The hydrogen bond and the various contexts in which the hydrogen bond functioned in the educational experiments are discussed in Section 6.3. The closing section reflects on the educational experiments and on teaching chemical structures. In this section, outlines for an educational structure for chemical bonding are presented (Section 6.4).

6.1 Adjustments for a Second Experiment

In the cyclic procedure of research and development, the preparations for a second educational experiment are twofold: first, the results of the previous experiment lead to a better insight into how to carry out the next experiment; and, secondly, the educational text is revised in light of these results and the objectives of the experiment.

To begin with, I give an account of an adjustment that was made in order to gather research material on drawings. I present the reasons for looking for a new design of the closing episode as part of the global context (6.1.1). Subsequently, as the 'openness' in assignments appeared to cause difficulties in some cases, I go into the problem of how to 'regulate the openness' in assignments and also in the text. I give examples and go into the changes made to the first three assignments (6.1.2). Then, I discuss the meaning of dashes in the structural formulae using correspondence terms and contexts. The adjustments to some assignments and reasons why other assignments were not changed, are listed (6.1.3).

6.1.1 Global context, communication and closing episode

In the global context of creating knowledge, I regard communication and opportunities for discussions as important factors. In a previous section (5.4) I mentioned the

possibility of a dialogue with the text. The parts of the first version of the narrative I considered to be most conducive to dialogue were the assignments. However, looking more closely at the description of chemistry practice given in the introductory part of the educational text revealed that there was another possibility for communication resulting from working with the text and that this possibility could provide research material.

Communication among chemists as described in the introduction of the educational text can be divided into three types: 'internal' communication in a personal lab journal; direct communication in discussions with others and through lectures; and communication at a distance with the outside world through papers and books. An analogous division into three types can be proposed for communication among students. For instance, the report of an experiment or the written answers for assignments can be classified as communication at a distance (with the teacher), and talking in small groups in the classroom as direct communication. In the framework of the educational experiment, the written reports and the tape-recorded discussions were available as research material (cf. Section 5.4). However, in the first experiment, internal communication was not explicitly provided for. Of course, students are expected to make notes while doing experiments, but initially these were not considered to be part of the research material. During my observations of the classroom discussions I realized that students' reports did not show the drafts of structural formulae sketched *during* the discussions, although sometimes students allowed me to make copies of pieces of scrap paper. To help me collect the drawings and notes produced during the small group discussions, I asked the students in the second experiment to keep group lab journals (internal communication in the group). Material gathered by means of these journals will be presented in Section 6.3.

The global context of creating knowledge as a human endeavour which has to be borne in mind when reading the narrative, contains aspects relevant to communication. In episodes of the narrative, the biography of the substances is also told as the story of people creating knowledge unfolds. The communication function of the narrative is essential for providing this information. To give the information in a consistent manner, the episodes should not only show internal coherence but the transitions between the episodes should be also coherent. When revising the narrative I took care to mention the person, the place and the period of the action in each episode in the framework of people creating knowledge. I also tried to standardize the transition by closing each episode with a remark on what had been established so far of the relationship between structure and properties and by looking ahead to the next step as regards the sequential contingency. For instance, the Lewis episode ends with the assignment on the hydrogen bond *within* molecules in the first version. In the revised version, I look ahead to the next episode by adding a remark on hydrogen bonds *between* molecules, with which other properties might be explained.

In the first educational experiment, the results of the closing episode were disappointing for various reasons. The episode gave examples of the use of maleic acid and fumaric acid in society or industry today. The transition from the foregoing episode to this closing episode included a review state of affairs to date and a comment anticipating the next episode, but both were formulated in general terms. The beginning of the closing episode showed no link with other episodes, because no person and no place were mentioned, and no reference was made to publications.

Furthermore, there are so many applications of the two substances that I found it difficult to make a selection, and consequently, I offered an overload of information. No experiments about societal or industrial issues were included and the experiment with the reaction mechanism appeared to be more relevant to an earlier episode on questioning the meaning of the representation of the double bond by two dashes (Section 5.4). I concluded that in the closing episode, the basic assumptions underlying the design of the episode and the selection of the appropriate chemistry content were not clear enough and apparently not in accordance with the guidelines for recontextualization used to design the other episodes. No questions were asked which could have guided the process of searching out suitable chemical topics and, subsequently, incorporating them into an educational text with the desired global context of creating knowledge.

In Section 6.2, I discuss the design of the revised version of the closing episode and the questions which provided guidance for developing the design.

6.1.2 *Regulating the openness*

The 'open' assignments were intended to enable students to gain experience in handling conflicting information and making decisions about various interpretations of this information. The results were contradictory. First, it appeared that the open character, the openness, should not be restricted to certain assignments only, but should be incorporated in other assignments and in the main text as well, to give more opportunity for discussion and decision-making. Therefore, I adjusted the educational text to enhance the open character of the other assignments and the text. But then the openness had to be regulated, because in the educational experiment, the results of the titration experiment, for example, made it clear that the text should not be too open: students need some certainties to hold on to. This resulted in offering the information in the text and in the assignments in a less 'open' way, in a *more specific* way. Some assignments are more structured and contain more specific sub-questions. But this should not be at the expense of a certain degree of freedom. Therefore, some statements were made more 'open', *more relative*, to stimulate the making of choices and decisions.

As mentioned above, the measures to enhance the openness were extended from the assignments which were already 'open' to other assignments and also to the textual parts of the narrative. I give examples of what is meant by 'more specific' or 'more relative' by comparing the first version of the educational text with the second version (see Appendix for the second version).

The first example is from an assignment formulated as follows in the first version:

Assignment (4)

Calculate the molecular formula of 'water-free' maleic acid using Pelouze's results. Using structural formulae, show how this compound can be formed from maleic acid.

In the revised version the assignment is:

Assignment (5)

Calculate the molecular formula of 'water-free maleic acid' using Pelouze's results, and draw up a structural formula.

Does this structural formula help you to choose which structural formula belongs to maleic acid? Explain your answer.

In the first part of the new formulation, the assignment is more specific in that it asks students explicitly to design a structural formula. In the second part, the authority to make a decision is with the student. This I call more relative. Whether the answer to the question on structural formulae is regarded as 'correct', might depend on the argumentation, thereby providing the opportunity to discuss the decisions in the classroom.

Another example of more relative and more specific is from the Yardley episode: the first version:

We explain and predict properties of compounds with the aid of the structural formulae designed.

and the revised version:

The properties of other compounds can be understood and predicted with the aid of the knowledge of molecular structures thus obtained.

The decisive formulation in the first version is replaced by a more relative expression of a possibility. On the other hand, the information is less open by mentioning molecular structures and by referring to "other compounds" instead of to compounds in general.

A third example is a fragment of the text which precedes the data of the quantitative analysis by Pelouze:

What formula can we write for the acid? A conclusion of experiment 3 is that the compound contains at least hydrogen and carbon. Pelouze assumed that, in addition to these, it contained only oxygen. The empirical formula can be calculated by carrying out the elemental analysis quantitatively. About 1830, Liebig (...) developed a method for this purpose.

The revised version reads:

Around 1830, Liebig (...) developed a method for carrying out similar experiments quantitatively. Pelouze therefore knew how to work out the empirical formula of a chemical compound. He assumed that the acid he was investigating, (...), contained only oxygen in addition to carbon and hydrogen.

The experimental results in this part of the story are related to persons. Students can accept the results presented but these results can also be discussed for their relevance in the students' work.

The above-mentioned examples show how information was made more specific or more relative than in the previous version.

An assignment which is made more open, is the first experiment in the educational text, i.e. the formation of white crystals in a test tube. I mentioned in Section 5.5 that students taking part in the educational experiment were not much interested in the new substance and the descriptions of its properties. On the one hand, this is not surprising in view of the current school practice of learning formulae and referring to substances only as illustrations of the formulae. On the other hand, the steps taken to draw attention to the substances turned out to be ineffective, one of the reasons probably being that the experiment was not carried out by the students themselves. They should gain more experience with the substance themselves, in accordance with the guiding principle of starting from the substance.

Therefore, I considered it important to make adjustments to the text to ensure that students really do get acquainted with the white solid. The experiment in the revised version was changed so that the students perform the dry distillation of malic acid themselves. They heat a test tube filled with an amount of malic acid over a small flame of a gas burner in the fume cupboard. Depending on the temperature during heating, either fumaric acid or maleic acid is formed, or both. The circumstances of the heating as described above are most likely to favour the formation of fumaric acid (Pelouze, 1834).

Subsequently, the students are asked to investigate some properties, for instance solubility in water, of the substance they had made themselves instead of just using the school supply. They perform a qualitative elemental analysis with their own sample. The findings from this sample have to be compared with the data of the two substances Pelouze reported on. Then, students can try to decide if their substance corresponds to one of the two isomers. The relative uncertainty of not knowing which substance is formed and the essential decision-making, are regarded as appropriate in the design of the educational text.

As more material is needed to determine the molar mass, students will not have enough of their own product. Only when this stage has been reached should the school supply of the substances be used. This has its advantages for the teacher and for the students themselves because the results of the titration experiment for instance, are more reproducible, and the results of all groups in the class can be compared because they used the same substances.

The adjustments of the first three experiments, i.e. the preparation of one's own sample and deciding on its properties, could be regarded as more relative, thus enhancing the openness.

The titration experiment called for the opposite approach, i.e. of restricting the openness. Two assignments have been designed instead of one structured by prescribing

the sequence of the experiments and the order in which the two indicators should be used. The titration of Pelouze's acid (maleic acid) is carried out before the titration of moss acid (fumaric acid). The indicator phenolphthalein is used first and then methyl orange. By performing the titrations in these structured sequences, comparing and discussing the results of the titrations can be carried out in a more specific way.

Another assignment which was made more specific is the one in which hydrogen bonds are used to compare the various acid strengths of the carboxylic groups in maleic acid and fumaric acid, and to explain the differences. The assignment on the hydrogen bonds is closely linked to the titration assignment. From an educational research point of view, the titration assignment is the focal point of the first two episodes in the narrative, and I regard the hydrogen bond assignment the focal point of the Lewis and Yardley episodes.

The hydrogen bond assignment is prepared in the preceding part of the Lewis episode on the meanings of dashes. I discuss these meanings in relation to the sequential contingency of the molecular structure theory in the next subsection.

6.1.3 Structural formulae, dashes and sequence of contexts

The results of the titration experiment led to a description of various contexts. In 5.6.2 I presented a summary of a sequence of contexts in accordance with the sequence of episodes and I gave the possible meanings of dashes in structural formulae in the various contexts. In this section, I look further into this and describe some of the adjustments in the second version of the educational text which are relevant for the hydrogen bond assignment at the end of the Lewis episode in the narrative. In the Lewis episode, various meanings of dashes in structural formulae are presented. Some of these meanings refer to the model aspects of the structural formula while others refer to the representation of chemical properties (eg. acidity). By looking at the contexts in which the dashes have their meaning, the interrelationship of the concepts in the sequential contingency could be made clearer.

Throughout the educational text, the meaning of the dashes in a structural formula is becoming more complex, since layers of meaning are being added.

In the beginning of the educational text, the substance is represented by the molecular formula normally written without dashes. If written with dashes as a 'precursor' for a structural formula, the meaning of a dash in the framework of the educational text is 'belonging together'. The mass context is mentioned here since the empirical formula is drawn up as a result of experiments in the mass context. In the Van 't Hoff episode, the meaning is added of 'the closest distance in space'. The meaning of the dashes is then in the distance context, i.e. distance in a spatial sense. The meaning of dashes in the Lewis episode might, on the one hand, be regarded as a result of bookkeeping of 'two dots constitute a dash'. On the other hand it must be realized that the electrons in the dot representation are charged corpuscles and that bonding is explained in terms of

electrostatic attraction. The dash replacing two dots means 'a shared electron pair' in the charge context.

The interpretation of the dashes in a structural formula depends on the context in which the dashes and the structural formulae have to function.

In the educational text, the dashes in the structural formulae are given first one meaning, and subsequently others, *while retaining previously attributed meanings*. This is the case, for instance, in the Lewis episode. The various contexts in which the dashes have to function require a certain mental agility on the part of the students, who must be able to switch backwards and forwards between different contexts (thinking in the framework of the relativity of models), as well as the experience to enable them to decide which meaning is applicable. (It should be realized that the meaning of the characters as symbols in a structural formula changes with the changing meaning of the dashes (cf. 5.6.2). This is a complication that is related to difficulties with interpreting the dashes in the educational text.)

In the Lewis episode the introduction of the meaning of a dash as indicating a bonding electron pair is followed by a series of assignments in which layers of meaning are added. Experiences from the experiment with the first version of the educational text resulted in adjustments in the second version to adjust the openness, for example.

The meaning of the dashes is extended to a representation of chemical reactivity in conjugated systems, i.e. specific addition reactions, such as the addition of bromine to 1,3-butadiene. Assignment 8b in the first version of the Lewis episode was on drawing a structural formula with dots and dashes. Several students did not like drawing the many dots in the structural formula of fumaric acid, as I could conclude from student conversations and the written reports. However, I retained the assignment on replacing the dash by dots. I remained convinced that by using dots, more attention could be paid to the meaning of a dash as two electrons of an electron pair, and to the 'jumping' of electrons in representations of reaction mechanisms with conjugated systems.

The next assignment in the Lewis episode is on another meaning of the dash as a lone electron pair, followed by an assignment on drawing a hydrogen bond. A result from the first educational experiment was the decision to keep the assignment on the dative-covalent bonding of the Lewis acid-base theory and, also, not to specify how to draw a hydrogen bond. However, in interpreting students' drawings, one then has to be aware of the complication that some students will draw the hydrogen bond with a solid dash, and not with a dotted line, as is customary.

In the first version of the educational text, the assignment on the hydrogen bond consisted of a single sentence on explaining the difference in acid strength of maleic and fumaric acid using hydrogen bonds. Although the preceding assignments and narrative texts were regarded as sufficient preparation for this assignment, it appeared to be too open for students to get to grips with adequately. Therefore the assignment on the hydrogen bonds was more structured in the second version. In this assignment, as was

the case in the titration experiment, the openness was adjusted to enable the students to find their way in the discussions towards the objective, i.e the distinct use of dashes and dotted lines and their meaning.

I give an account of the educational experiment on the hydrogen bond in Section 6.3.

6.2 The Trial with Recontextualization

In this section I report on the design of the closing episode of the educational text. At first, I described my efforts as 'two translations' which I considered necessary in order to make educational material for school use about issues from chemical research and industry, with the educational objectives in mind. I will link the 'two translations' to educational analysis, decontextualization and recontextualization.

Compared with the first version of the closing episode, I restricted the choice of applications of fumaric acid to its role in the industrial synthesis of aspartame, and of maleic acid to the development of polymer chemistry.

Aspartame, a sweetener, is synthesized from L-aspartic acid and the methylester of L-phenylalanine in an enzymatic reaction to ensure the production of the desired isomeric structure, a-aspartame (the b isomer has a bitter taste). The synthesis of the first compound, L-aspartic acid, is carried out by using ammonium fumarate and immobilized *E.Coli* cells (Sato and Tosa, 1992). I regard this reaction as a beautiful example of a biocatalytic process with an efficient atom utilization (Sheldon, 1993, p.425; Van den Tweel, 1993, p.511). In the part of the closing episode on fumaric acid, the emphasis is on the spatial aspects of the structural formulae.

The importance of maleic acid in polymer chemistry (see the overview in Section 5.2) is related to various polymerization reactions carried out using maleic acid or fumaric acid as raw material. Because maleic anhydride is often used in polymerization reactions instead of maleic acid, I focus on the role of both, maleic acid and its anhydride, in the closing episode.

I analyze the maleic acid section of the closing episode as an example of a possible way to develop educational texts by searching, selecting and using new information.

I begin the search for suitable information in 6.2.1, and I continue with the selection of the relevant concepts for the closing episode (6.2.2). In 6.2.3, I comment on writing the closing episode. I discuss a relationship between the 'two translations' and the terms decontextualization and recontextualization, and I elaborate on possible global contexts for educational texts.

6.2.1 A question to guide the search

The search for information on a connection between the structure-property relations of maleic acid and the application of the acid in the polymer industry started with the following question: was the double bond or the presence of two carboxylic groups in the

structural formula of maleic acid a reason for chemists to suppose that maleic acid would engage in polymerization reactions, and if so, who tried that first?

With this in mind, I looked for a publication where using structure in such a way was mentioned and, because I was looking for the origin of the developments, the search was among older publications. During my search it became clear that looking for publications on structure was not going to further my search, at least not with regard to maleic acid. Meanwhile, I learned more about the developments in the history of plastics, although I was not intending to go too deeply into that. From survey articles (for instance, Staverman, 1986; and VNCI, 1993) I came across developments which were a result of a coincidental combination of circumstances (e.g. polymerization of ethene) as well as those which resulted from systematic chemical research into compounds in general. The chronological history of polymer chemistry shows a whole chain of crafts, techniques and empirical experiences. Theoretical assumptions were sometimes less of a help than a hindrance (cf. Zandvoort, 1988).

The answer to the first part of the question therefore appeared to be negative. The question was consequently reformulated as: *who was the first person (or one of the first) to associate maleic acid with a polymerization reaction?*

An early publication on the synthesis of a copolymer of maleic anhydride (MA) was found in the Encyclopedia of Polymer Science and Engineering and also in a compendium on maleic anhydride (Trivedi and Culbertson, 1982). The first person was probably Wagner-Jauregg (1930), who published an article on polymerizing addition reactions of two different low-molecular building blocks. In a sense he used information on structure when he pointed out the double carbon bond in these building blocks (Wagner-Jauregg, 1930, p.3213). He discusses differences and similarities between homo- and heteropolymerizations and between polymerization by addition and polymerization by condensation. Furthermore, he remarks:

"Polymerization reactions involving two ethylene compounds were investigated in this project, as examples of addition heteropolymerizations. One of the two ethylene compounds was always maleic anhydride. This compound does not show any polymerization tendency by itself, but is known for its addition potential (...)." (Wagner-Jauregg, 1930, p.3215)¹

After experiments with varying initial concentrations (p.3219), he then carried out elemental analysis. Wagner-Jauregg found that the product of the reaction of MA with stilbene (diphenylethene) must consist of alternating MA and stilbene units:

¹ "Als Beispiele für Additions-Hetero-polymerisationen wurden in dieser Arbeit Polymerisations-Reaktionen zwischen zwei Äthylen-Körpern untersucht. Der eine der beiden Äthylen-Körper war stets Maleinsäure-anhydrid. Dieses zeigt für sich allein keine Neigung zur Polymerization wohl aber ist seine ausgesprochene Additionsfähigkeit bekannt (...)." (Wagner-Jauregg, 1930, p.3215)

"These molecules appear to be formed by alternate linking of hydrocarbon to maleic anhydride by releasing the double bonds (...)" (Wagner-Jauregg, 1930, p.3216)²

Wagner-Jauregg was co-author of an earlier article on the addition of maleic anhydride to diphenyl substituted polyenes with conjugated double bonds in the framework of an investigation of dyes. An unexpected reaction was observed when stilbene, 1,1-diphenylethene, was found to react readily with MA although only one double bond is present:

"The reaction product which contains approximately 1 mol stilbene to 1 mol maleic anhydride, is amorphous and consists of large molecules. It is probably built in a chain form. It should be described in more detail elsewhere in conjunction with the addition of other ethylene compounds." (Kuhn and Wagner-Jauregg, 1930, p.2662)³

My interpretation of these publications is that the results of the investigations of addition reactions and reactions where polymers are formed, led to the assumption of a causal relationship between double bonds and polymerization reactions. *The knowledge which is now available in structural formulae did not inspire the investigations but was developed as a result of them.* Therefore, looking for early notions of a structure-property relation led to looking for the substance itself.

In both articles by Wagner-Jauregg, reference is made to the work of Diels and Alder. The names of Diels and Alder are associated with "the one reaction of maleic anhydride that has been investigated most in the last-half century" (Trivedi and Culbertson, 1982). This reaction of maleic anhydride with conjugated dienes, an example of the so-called Diels-Alder reactions, is of great importance for organic syntheses.

The answer to the question of who was the first is Wagner-Jauregg in his work on polymerization reactions. The work with maleic anhydride and conjugated systems by Diels and Alder is also worth mentioning.

6.2.2 A question to guide the selection

The question is, which concepts should be selected from the articles and why. I discuss this question in relation to the concepts introduced in the earlier episodes, and in relation to three criteria for recontextualization mentioned in Section 5.1: starting from the

² "Offenbar entstehen diese Moleküle durch abwechselnde Aneinanderreihung von Kohlenwasserstoff an Maleinsäure-anhydrid unter Aufhebung der Doppelbindungen (...)" (Wagner-Jauregg, 1930, p.3216)

³ "Das Reaktionsprodukt, welches auf 1 Mol Stilben annähernd 1 Mol Maleinsäure-anhydrid enthält, ist amorph und hochmolekular. Es ist vermutlich kettenförmig gebaut und soll an anderer Stelle im Zusammenhang mit der Addition weiteren Äthylen-Körper näher beschrieben werden." (Kuhn and Wagner-Jauregg, 1930, p.2662)

substance, the molecular structure theory and creating knowledge as a human endeavour.

From the above quotations it can be seen that the articles by Wagner-Jauregg are relevant for designing the closing episode of *Kennis Maken*. His work offers various links with the concepts and criteria of earlier episodes. For instance, the observations that certain special addition reactions are polymerization reactions, and the decisions taken on conflicting experimental results, could be considered from the point of view of creating knowledge. The relationship between structure and properties which can be recognized in his work fits in with what is said on addition reactions and conjugated systems in earlier episodes, and is therefore relevant to the molecular structure theory. The possibility of using the experimental results of the elemental analysis, especially when a decision on an alternating copolymer has to be made, fits in well with the aim of taking the substance itself as starting point in the narrative.

The passages selected from the work of Diels and Alder are also linked to the knowledge of maleic acid in the earlier episodes of the narrative, such as the assignment with butadiene and the 1,4 addition reaction. Diels and Alder (1928, p.102-103) came to the conclusion that maleic anhydride and maleic acid react, through an addition reaction, quite easily with cyclobutadiene and butadiene, and also with more complex hydrocarbons with systems of conjugated double bonds. They continue:

"The double bond of the said unsaturated anhydride or acid opens up, and, in all cases, a linking takes place of the free valences in the 1,4 position on the hydrocarbon under consideration, in which a new double bond is formed between the carbon atoms 2 and 3." (Diels and Alder, 1928, p.103)⁴

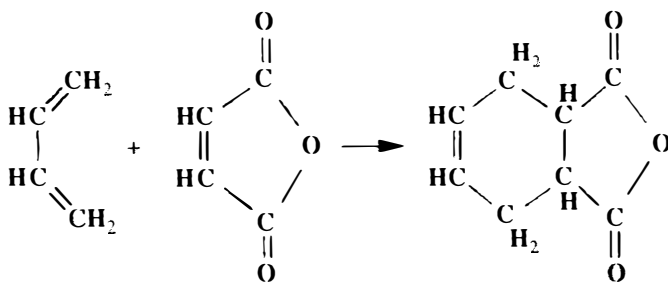


Figure 6.1 A Diels-Alder reaction

⁴ "Die doppelte Bindung der genannten ungesättigten Anhydride oder Säuren öffnet sich, und es kommt in allen Fällen zu einer Angliederung der freien Valenzen in 1,4-Stellung an die betreffenden Kohlenwasserstoffe, wobei sich die neue Doppelbindung zwischen den Kohlenstoffatomen 2 und 3 bildet." (Diels and Alder, 1928, p.103)

The drawings with more complex hydrocarbons, for example cyclopentadiene, are difficult to make because three dimensions of the resulting spatial structures must be drawn two-dimensionally. Therefore, discussions among students are to be expected.

In order to select the information for the closing episode, more publications and books were studied than mentioned here. A compendium such as *Maleic Anhydride* (Trivedi and Culbertson, 1982) is useful when fitting in new ideas requires a check on the chemical information.

The selection of the format for the closing episode was determined by the consideration that it was to be the final episode of a narrative to be used at school. As the educational experiment in the classroom took place just before the final exams, the design could have the format of an assignment as in the exams, i.e. short texts providing information alternated with questions. This format was also chosen because students could regard this part of the educational text as a means of revising what they had learnt earlier.

Although the content of the closing episode on maleic acid is presented in the framework of a scientific chemical theory, I included the connection with current chemistry by mentioning the importance to industry of polymerization with maleic acid and the Diels-Alder reactions. For instance, the Diels-Alder reactions are used for synthesizing pharmaceuticals and agrochemical compounds, i.e., specialty products. The maleic acid polymers, such as SMA (a copolymer of styrene and maleic anhydride), are widely used, as are the polymers which are formed by polycondensation reactions. This offers another opportunity to point out the use of the various meanings of structural formulae once these meanings are learned.

6.2.3 A question to guide the writing

When writing a new text, material has to be selected according to the objectives of the text. In the case of the closing episode, the question which would yield the guidance was obvious because the main objective of the educational experiment was to investigate how to teach the idea of the relativity of models. Various elements which had to be included in the educational text to achieve the objectives were indeed known: names of persons and periods of publication to be mentioned, and findings published in articles and books to be presented for discussion. Conflicting information should be given so that decisions are not self-evident. The concepts to be introduced should be connected to the molecular structure theory.

However, while writing the closing episode I realized that although all the elements required in the text appeared to be present and correct, the result did not fit in with the earlier episodes. It took me some time to realize that the context in which the episode was written was different from that of the preceding episodes. I learned that, going from chemistry practice to chemistry for an educational text yet a different approach was needed; the content of the text was correct, but the manner in which it was presented

needed to be adapted to fit into the framework of the earlier episodes. Two translations were needed: one to turn chemical knowledge into chemical concepts suitable for teaching purposes, and another to incorporate these concepts into an educational text about the creation of knowledge as a human endeavour. *My experience with writing the closing episode was that specific measures, i.e. regulating the openness, were required to adapt the material so that it fitted in with the global context.*

These 'two translations' correspond to the ideas of decontextualization and recontextualization set out in Section 4.4 for the narrative. Selected concepts from chemistry practice are taken out of their context or decontextualized, but can still be arranged in a sequence which is meaningful for chemists. The first 'translation' could produce a correct chemical text with concepts organized linearly in a form which chemists will be able to understand. If no new context is provided, students no doubt will interpret the concepts in a context in which the concepts seem meaningful for them. This context might be that of school chemistry or everyday experiences (or a mixture of both), but not the intended context of, for instance, chemistry as a science. Whatever context is intended, a second 'translation' should build it into a suitable context, i.e. recontextualize it. In this respect, it is not only the *choice* of the global context that is important but also how it is worked out. In the example of recontextualization given here, the regulated openness introduced proved to be a significant factor in successfully building the concepts into the global context of creating knowledge as a human endeavour.

To conclude this section on the closing episode, I discuss three possible global contexts in relation to the first and second version of the closing episode. Exploration of current chemistry is necessary to find suitable topics for chemistry education. It is not enough to choose appropriate concepts: a *design* for the global context in which they are presented must be chosen as well. This context could be the context of scientific practice, or of industry, or of society. But the meaning of the concepts to be taught varies according to the context in which they are used. The meaning of 'pure water' in the scientific context differs from the meaning of 'pure water' in the industrial context and 'pure water' in the societal context. This implies that more must be known of the requirements for designing educational texts within the chosen global context. Further educational analysis is needed to identify these requirements. The educational analysis must be extended to examine the compatibility of the chemical concepts chosen with the chosen global context.

I call the global context for scientific chemistry 'creating knowledge' (cf. the title of the educational text, 'Kennis Maken'). Similarly, the global context of industry might be called that of 'creating wealth' or 'making money', since arguments and decisions are ultimately made on basis of the economic profitability of the processes and the products. If societal issues are to be taken into account, the global context of society could be seen as the 'creation of quality'.

An important development regarding global contexts for different types of 'creating' or 'making' is investigated by Van Aalsvoort in her work on designing an educational text on the theme of 'preparing products' (cf. Van Aalsvoort, De Vos and Verdonk, 1994).

I end this section with a remark on the usability of the educational texts with regard to the recontextualization. The effectiveness and suitability of the concepts and the global context chosen can only be evaluated after experimenting with the educational texts in cooperation with students and teachers. I reported on such an educational experiment in the previous chapter, i.e. the titration assignment. In the next section I report on the educational experiment with the assignment on the hydrogen bond.

6.3 The Trial with the Hydrogen Bond

In this section I present the results of the assignments on hydrogen bonds in the educational experiments. Since the students learned about hydrogen bonds in previous years, the educational text aimed at providing enlargement and deepening of insight.

I show from experiments with the first and second versions of the educational text that students depict the hydrogen bonds in various ways and that these depictions can be interpreted as belonging to different contexts (6.3.1). I report on the educational experiment in which two groups of students were working with the second version of the educational text. I present a transcript of the discussions on the assignment in which students are asked to explain the differences in the acid strength of maleic acid and fumaric acid by using hydrogen bonds in structural formulae (6.3.2).

6.3.1 Hydrogen bonds depicted

As I mentioned before in Section 5.3.3, Lewis (1923) proposed a description of the hydrogen bond. In his view, the hydrogen bond between water molecules is *the hydrogen atom* which is attached to two oxygen atoms of different water molecules. In contemporary chemistry the hydrogen bond in water is usually depicted by a *dotted line between* a hydrogen atom of one water molecule and the oxygen atom of another water molecule. This line is interpreted as an attraction between the hydrogen atom and the oxygen atom. (The hydrogen atom of the hydrogen bond in the Lewis sense looks like a bridge between two oxygen atoms. In the Dutch language the 'bridge' notion is present: the hydrogen bond is still called 'waterstofbrug' or 'hydrogen bridge'.)

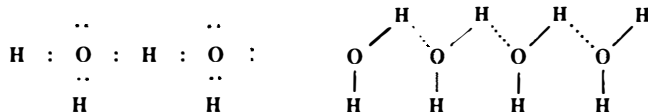


Figure 6.2 Lewis' conception and a contemporary interpretation of a hydrogen bond

A drawing made by students in the first educational experiment could be interpreted as depicting the hydrogen bond in the Lewis sense, see Figure 6.3. The students had to indicate the hydrogen bond between a hydrogen atom of one water molecule and a free electron pair of another molecule.

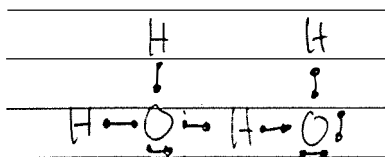


Figure 6.3 A students' drawing of a hydrogen bridge

The students first worked with dots for valence electrons and then made dashes of the dots. The recognizable dots make the drawing look like Lewis' conception of the hydrogen bond. My interpretation of the hydrogen bond in this drawing is that it is seen as a hydrogen atom. These students did not use their previous knowledge of the hydrogen bond as a dotted line. In this case, they might have been misled by the previous assignment (assignment 9 in the first version) in the educational text on the dative covalent bond. However, another interpretation is possible, *viz.* that the students intentionally made the drawing this way by using the definition of the hydrogen bond from a textbook used earlier. There, it is explicitly stated that the hydrogen atom constitutes a "bridge" (CHEMIE 4V, 1984, p.96). In this method of depicting the hydrogen bond, the exception to the usual valence rule for hydrogen is made more visible than in the drawings with dotted lines.

In the following I focus on the dotted line depiction of hydrogen bonds.

Which meaning do students attribute to a dotted line in their drawings of hydrogen bonds? My first experience with meanings of dotted lines interpreted in various contexts was during a small group discussion of students working with the second version of the educational text. Here is a summary of the notes I took:

Group 4 was busy with assignment 11 on a hydrogen bond between two molecules of water. As they used a new page (*i.e. in their journal*), assignment 10 was not in sight. Not knowing how to proceed, they called the teacher for help. The teacher gave a hint (*in a drawing*) of delta plus and delta minus, knowledge from earlier years. "Oh, is that what they mean". The students made a new drawing of two water molecules (with what was almost a right angle between the two bonds) and drew a dotted line from H of the first molecule to O of the other molecule. Then I asked them whether they could draw a hydrogen bond between the water molecules with dashes (*i.e. showing the non-bonding electron pairs*). Their answer was to draw a dotted line from the H of the first molecule to the O of the other molecule next to the dash.

The dotted line ended at the end of the dash that depicted a lone electron pair of the oxygen atom. A copy of the drawings from the group lab journal of the students is shown in Figure 6.4. The drawing in Figure 6.4a is made by the teacher, and the other two Figure 6.4b and c are students' drawings.

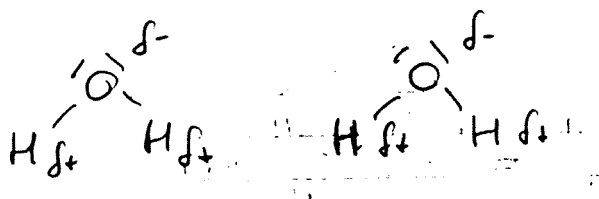


Figure 6.4a

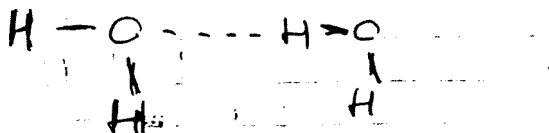


Figure 6.4b

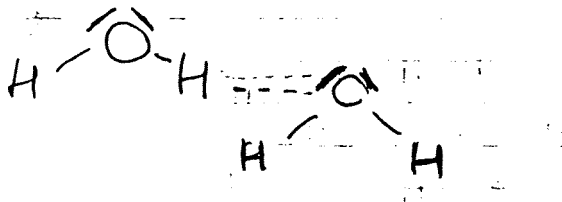


Figure 6.4c

In the original drawings, a dotted line in pencil was drawn by me towards the centre of the dash of the electron pair of an oxygen atom. In the copy, this line is barely visible. The students and I were engaged in a discussion on dotted lines between the water molecules and on the 'correct' position of the dotted line. The discussion came abruptly to an end as the lesson ended. I had no opportunity to ask the students what they meant by the position of the dotted line.

However, when looking at the drawings and analyzing them together with the teacher, I realized the possibility of two interpretations of the dotted lines used to depict hydrogen bonds. In the drawings I recognized two different contexts in which the hydrogen bond can be meaningful. The first is a charge context with a delocalized charge distribution depicted as delta plus and delta minus. The second is a context of counting the electrons and representing the shared and lone electron pairs as dashes in an application of the rule of two and the octet rule.

This experience enabled me to see meanings of dotted lines depicting hydrogen bonds in relation to the meanings attributed to dashes in structural formulae (cf. 6.1.3). The dotted line might mean 'belonging together' as in a mass context, or it might convey the meaning of a certain distance in a spatial sense, and it might stand for an electrostatic force of attraction as in a charge context. However, *within the charge context the meanings can co-exist* (i.e. adding layers of meaning). Therefore, within the charge context, a dotted line might mean just the electrostatic attraction of belonging together, or a delocalized but spatially separated distribution of charges as mentioned above, with notations of delta plus and delta minus. Or, it could be associated with discrete charges when ionic notations are used, as for instance with a hydrogen maleate ion. The students' drawings of Figure 6.4b and c show the charge distribution of delta plus and delta minus. However, the meaning of the dotted line *next* to the lone electron pair dash might just mean belonging together, or it could be interpreted as revealing uncertainty about the meaning of the lone electron pair dash.

The group of students who, at first, could not answer the question of the assignment, did recognize a hydrogen bond in the charge context, but time did not allow them to tell me how they might have combined the 'counting the electrons' context with the delocalized charge distribution. They showed me, however, how I could distinguish between interpretations in various contexts. I could use this experience to interpret results from the educational experiment with the hydrogen bond assignment.

6.3.2 *Hydrogen bonds oriented in space*

In the educational experiment with the second version of the educational text, the assignment of the hydrogen bond deals with explaining the difference in acid strength of maleic acid and fumaric acid. The aim of the assignment is to use structural formulae (or parts thereof) with and without dotted lines, and subsequently to explain why maleic acid *with* an intramolecular hydrogen bond will be a stronger acid than *without* such a bond.

Assignment 12 in the second version of the educational text reads:

a. Demonstrate the possibility of hydrogen bond formation within the maleic acid molecule.

What effect do you think this would have on the dissociation of the other hydrogen atom as an ion?

b. Show where a hydrogen bond could be formed in the hydrogen maleate ion.

What effect would you expect this to have on the dissociation of the second 'acid' hydrogen atom?

c. Answer the same questions for fumaric acid.

d. Explain the possible differences in acid strength as found in the titration experiments 4 and 5.

Two small groups of students were occupied with this assignment during an educational experiment. Two members of one group, Rh and Ta, discussed the assignment while drafting structural formulae in their group lab journal. They were joined by Cr from the other group and by me, G, in case they wanted advice.

Transcripts of the recorded discussions and copies of the drawings are given below.

Transcript Assignment 12

- 1 Rh Maleic acid molecule
Do you think we could have a hydrogen bond here?
- 2 Ta O, H
- 3 Rh Don't think so, what about the other one,, the hydrogen maleate
- 4 Ta (?)
- 5 Rh But how
(...)
- 6 Rh The other one, you mean
Miss, (...)
- 7 Rh I don't think hydrogen bonds can be formed here, in maleic acid

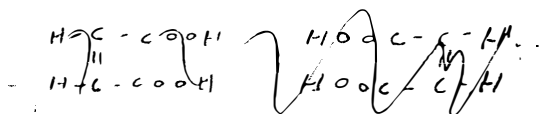


Figure 6.5

- 8 G All right but how do you normally draw a structure. So if you here, what is it called. Look
- 9 Rh Look here, this is also apart
- 10 G Write it down properly, I mean, that, that. It does not work, you're quite right. Go back one step and look how I did it, with hydrogen bonds. Mr. Lewis thought we should draw the hydrogen bonds, if you have written down which electron pairs
If you say that you can't do it this way, just try drawing a structure with all the free and shared electron pairs.
- 11 Rh I'll try
Using the OH group
- 12 G That is often the problem with questions
- 13 Rh Here we have
- 14 G That's brilliant
- 15 Rh As such
H here, H here.

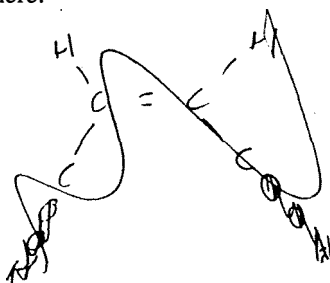


Figure 6.6

- 16 Ta Just draw the acid group
 17 Rh Why, yes of course, separate
 18 Ta Not a bad idea, look then the O is
 The O has two electron pairs
 19 Rh Patience is a virtue!
 A real shitty test
 20 Ta But fun
 21 Rh Mastermind. Here you draw two and there you put two
 Here we we draw one and we draw one, no that's not right, then we have
 five

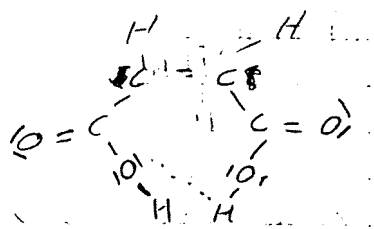


Figure 6.7

- 22 Rh But now he's got one. Two, three, four, that's enough
 23 Rh This one will attract that one, or something
 24 Rh Draw it this way
 25 Rh Maybe I could do something, in a molecule
 26 Rh Look, what about this. This, this one going here and that and that
 27 Cr If you draw this thing here, then the H gets the bond
 28 Rh Then you get this, the H goes here, that H goes underneath. Look, this way,
 ssssss
 29 Cr This O will attract two Hs, instead of just one H. So it'll attract both, but
 not so strongly I mean and it is easier to get that other one out, if you just
 30 Rh I don't think so. I guess the bond will stay just as strong
 31 Cr No
 32 Rh Because this one is attracted by these two, they have no influence on
 those
 33 Cr But it should, be
 34 Ta But this one is less acidic, isn't it. That's OK then
 The other one has less possibility of a hydrogen bond
 35 Sr No, this one is acidic
 36 Ta More acidic
 37 Cr Maleic acid is more acidic then, hydrogen maleate is less acidic
 38 Rh That's logical. That's logical, in itself
 39 (?) (?)
 40 Ta It can form hydrogen bonds, and then it is more acidic?
 41 Rh I don't really understand
 Miss
 42 Rh We could do away with this, in couldn't we. It attracts here doesn't it. O
 attracts that H, for instance
 43 G Yes

- 44 Rh But why is this molecule more acidic than fumaric acid? Why does it, split off more easily?
- 45 G Think of something
- 46 Rh But what did he say
But what did he say that O also makes that H attract stronger so to speak, to that H (?). But I think that is not true
- 47 G Because
- 48 Rh Because these two have nothing to do with that bond
- 49 G Which two
- 50 Rh These two, these two electron pairs have nothing to do with that electron pair, don't they?
- 51 G All right. Then, if you look at it this way, then
- 52 Rh Is it in(?)
- 53 G Just a moment, concentrating, that is a real problem. If you use this it looks like you can't work it out, yes

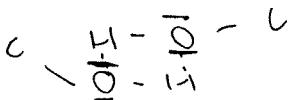


Figure 6.8

- 54 Rh What I was just thinking is if you get this from that, and this goes underneath, so OH. That H goes to that
- 55 G Goes underneath, so you have to, under the paper
- 56 Rh And this here that C comes from there, so, so. And then it has formed two hydrogen bond. But, yes, it seems rather strange
- 57 G But eh, why do you think it is strange. Because those hydrogen bonds, Lewis drew them towards the lone electron pairs. The question is do we still do it the same way. But to the lone electron pairs
- 58 Rh These are here and here
- 59 G Yes. Couldn't you here, with what you're drawing now
- 60 Rh That could be so and so, so
- 61 G But why do you say that is rather strange
- 62 Rh Then it forms two hydrogen bonds. So it would be much less acidic
- 63 G It's a stronger acid
- 64 Rh It's a stronger acid
- 65 G So, one should always look what is observed, it is a stronger acid
- 66 Rh So it's not right
I really do not know how it splits off H⁺
- 67 G So, then you would say if I only look at the hydro, at the hydrogen bonds, then I can explain why hydrogen maleate is a weaker acid, that is
- 68 Rh Yes, but not explain why maleic acid is a stronger acid
- 69 G I think that is very good conclusion. I myself think it is logical
- 70 Rh But it does not fit
- 71 G But why not
- 72 Rh It is a stronger acid

- 73 Rh But, looking at the hydrogen bonds, maleic acid should be a weaker acid
- 74 G Well weaker, I don't know about that. But, the hydrogen bonds. You say you really cannot explain with them. If I look at the hydrogen bonds drawn between H, dotted line to a lone electron pair, I cannot explain why maleic acid is a stronger acid than fumaric acid. Have I summed it up correctly?
- I think that's very good. But now you say it does not fit because. Agreed, that is also a good one
- 75 Rh So you should have to somewhere else
- 76 G Could be, that could mean that explaining with hydrog
- 77 Rh Impossible
- 78 G It's not such a good idea here, because you say you can't explain. I do not know whether Ta agrees?
- 79 Ta Well, I wonder if that molecule really can be that way, because
- 80 Rh Then, should be more turned inwards here
- 81 G No, no, that's something
- 82 Ta If it really stays this way, then you could say, from here the H is pulled further away from this and then more in this direction. And then this bond would
- 83 G Look, what you really need to do is with molecular models and all the distances they found. You can see that in the next section, there are all sorts of distances that is about crystallography, all those distances. Then you can see that an awful lot was measured. Every time they were trying to see if they could get to know more. They do not come all that close together. Everything is rotating, this C-C, these two C-C's, there is that free rotation. This is not really a flat molecule, that's flat, but here that's all in the plane surface. That's according to the measurements. And furthermore as soon as you have right angles here, then you should take care, I think
- 84 Rh Yes, but they have an effect on each other
- 85 G Yes all right, but I take care. Tetrahedron. I think if you say you can't work it out with the hydrogen bond, then that is reasonable enough. And if you say you want to explain it then you have to think of something else. D'you have to?
- 86 Rh Yes
- (...)

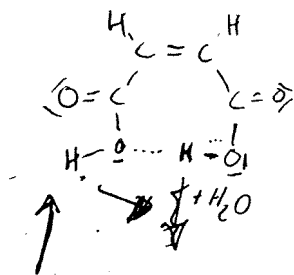


Figure 6.9

- 87 Ta If this one here is like this, then that hydrogen bond is here
 88 Rh O, the other one on the other side
 89 Ta Then that should, here, pull that H away from this O. Well not pull it off straight away, but more, but it will be weaker, then this bond will stretched out longer, then it should, this H should split off more easily, I think
 (...)

90 Ta That other O, that other O
 91 Rh That other H, with this one. Look what you, perhaps that's how it is. Then this one should be bonded in a normal way
 92 Ta This should
 93 Rh This, here's a half, you say, thus this plus H₂O, this goes away, you mean, and what then? Could you possibly get this
 94 Ta Other (?)
 95 Rh The other, more difficult ones split off
 96 Ta So the other one can too, no
 97 Rh Oh, this one goes this way
 98 Ta Then you have the same as (?)
 99 Rh No there is something wrong here, because this one is much more strongly bonded, but that, perhaps that it really does split off, because this one and a half, look this one is held one and half times as tight as this one

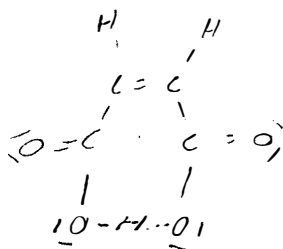


Figure 6.10

- 100 Ta (?)
 101 Rh We got to go to this other lesson. Look and this one, it can, it is really hard for this to split off. I think you are dead right, man
 102 Ta Why should it really be hard for this one to split off?
 103 Rh One and a half bond, this one, one plus a half, one and a half
 104 Ta This one is being drawn out
 105 Rh No, probably, this one is split off. Like just a, normal acid, like
 106 Ta We did conclude that it splits them both off, otherwise it would not work out with $n = 2$ and $n = 4$
 107 Rh Yes but not so easily, because it is a weaker acid than fumaric a, eh, or this one is weaker than hydrogen maleate or something

- 108 Ta No this one is a stronger acid than
109 Rh Yes this is stronger, this fumaric acid, but it is weaker than fumaric acid, marea
110 Ta Your'e right. Then this one should split off more easily and this one less easily
111 Rh Then this one should split off. Big deal!
112 Rh (?)
113 Rh He's got it. He's got it!

The students engaged in the discussion on hydrogen bonds were trying to explain the acid strength of maleic acid and hydrogen maleate with hydrogen bonds by comparing this with the acid strength of maleic acid and hydrogen maleate thought without hydrogen bonds.

My interpretation of this discussion focuses on the handling of the hydrogen bond and the meaning given to the dotted lines, and consequently also the meaning of the dashes.

Figures 6.5 and 6.6 show that the way in which something is drawn can obstruct the argumentation. The carboxylic groups must be drawn with distance depicted in a spatial sense if the possibility of relating atoms of various groups to each other is to be recognized (cf. lines 9 and 17). Figure 6.7 shows the hydrogen bond drawn with a dotted line between the hydrogen atom of one carboxylic group to an oxygen atom bonded to the hydrogen atom of the other carboxylic group (and not to the carbonylic oxygen). Although Rh was talking in terms of attracting (cf. line 42), his assumption was that by having two hydrogen bonds the hydrogen atoms will stay with the oxygen atoms and that maleic acid with hydrogen bonds is a weaker acid (line 62). In my interpretation of the drawing in Figure 6.7 the meaning here, and also in figure 6.8, is of atoms 'belonging together'. Despite remarks by Cr (cf. lines 27 and 37), Rh concluded that, by assuming the presence of hydrogen bonds, maleic acid has to be a relatively weak acid. Although he repeated my assertion (lines 63 and 64) that looking at the titration experiments reveals that maleic acid is a rather strong acid, he was not convinced of the need to change his conclusion. He reached the opposite conclusion and wrote this down into the group lab journal. Meanwhile, Ta went on trying to find a more satisfying explanation that fitted in with their experimental results. He was occupied with trying to argue on the basis of positions in the molecule (cf. lines 79, 82 and 87). According to his remarks, one OH group in Figure 6.9 was drawn in another direction when compared to the OH groups drawn in Figure 6.7. The spatial meaning of the dashes was used to change the drawing of the structural formula. Ta attributed a new meaning of attraction to the dotted line (line 89). He assumed that when one bond is getting stronger, the other has to be weaker. This might be a stronger and weaker attraction in the electrostatic argument from the charge context. Another interpretation might be that the stronger pull of one corpuscle implies a weaker pull from the other, without specifying of what stronger or weaker might be.

By assuming a different orientation for the OH group, both students, Ta and Rh, used the hydrogen bond to explain the acid strength of maleic acid (cf. lines 89 and 93). They were satisfied with the drawing shown in Figure 6.10 representing the weaker acidity of hydrogen maleate when a hydrogen bond is present (cf. line 99). It must be remarked that they did not include the negative charge of this corpuscle in the structural formula.

Since the students could reconsider an earlier decision because of experimental results and could give another meaning to a dotted line and a dash in the structural formula, I conclude that they were able to change contexts and therefore that they created knowledge in the framework of the relativity of models.

6.4 Reflections on Teaching Structures

In this section I discuss the results of the educational experiments reported here and in the previous chapter in relation to the research question about teaching and learning how to work with models of molecular chemical bonding. As a result of the educational analysis of chemical bonding and the introduction and use of models, the relativity of models was formulated as an objective for education in chemistry as a science, and especially for teaching chemical bonding from a pluralistic conception of scientific theories. The educational text designed for this purpose was intended to give students the opportunity to experience not only getting acquainted *with*, but also creating knowledge *in* chemistry as a science. To describe the creation of knowledge, I interpreted statements by Schwab about fluid enquiry and I will now use these interpretations to assess to what extent the aim of creating knowledge was achieved (6.4.1).

Then, I look at the chemistry content of the molecular structure theory in the text on chemical bonding. The second version of the educational text was adjusted by explicitly taking into account the sequence of mass, distance and charge contexts (cf. Section 5.6.2). I relate the sequential contingency to the tentative educational structure for chemical bonding, and specifically the covalent bond in molecules (6.4.2). An approach for introducing the molecular structure theory in earlier chemistry education is presented in Section 6.4.3.

Next, I discuss another way of teaching chemical bonding, which involves taking reactions as the starting point, instead of substances (6.4.4). The last part of the section deals with some of the consequences of new educational texts for implementation in school practice, for teachers and teachers' education and for the writing of textbooks (6.4.5).

6.4.1 Teaching structure for creating knowledge

As a result of the educational analysis reported in Chapter 3, the question of whether students can acquire insight into how to work with models, was reformulated as: How can students gain an understanding of the relativity of models in the context of

chemical bonding. In order to answer this question, the educational text was designed in the global context of creating knowledge as a human endeavour. In my interpretation of fluid enquiry, I described the scientific practice of creating knowledge in terms of cognitive conflict, reflection, creativity and consensus (cf. Section 4.4.2). If an educational text is designed with that aim in mind, the material collected during educational experiments in the classroom should provide some data on the four aspects mentioned above.

My interpretation of the discussions about the hydrogen bond is as follows.

The students working on the assignment on the hydrogen bond were able to put their own decision up for discussion; in a sense they set up their own cognitive conflict. The students took time out for a discussion. To enter a discussion on something can be interpreted as reflecting on the issues involved. It is difficult to pinpoint the creativity which the students, or rather one of them, undoubtedly showed by suggesting another way to draw a structural formula. Eventually, they reached consensus on an answer to the assignment and they were satisfied with the result.

From this interpretation of the students' activities I conclude that their activities showed the four characteristics of fluid enquiry. *The objective of creating knowledge was achieved in the trial of the hydrogen bond.*

The question of whether they acquired insight into working with models can be answered as follows. *They could change from one context to another with regard to the meaning of the dashes in the structural formulae, and their activities showed an awareness of the relativity of models.*

To see whether these students could apply this awareness in other similar assignments, other educational experiments should be carried out. Within the framework of school practice, it was not possible to extend the educational experiments to this purpose at that time. More educational experiments need to be carried out to see to what extent these results of students activities which can be described as creating knowledge can be observed in other situations. Also research is needed to examine how assignments like the hydrogen bond assignment can be designed for other chemical concepts, and to what extent these assignments can be discussed productively by other students and their teachers.

Trials with various designs of the titration assignment showed that discussions similar to those reported in the previous chapter took place when the titration assignment was presented during workshops with teachers and educational researchers and to a group of student teachers. The assignment was used in a version adjusted according to the more specific, i.e. less open, design. I could use the findings of the earlier educational experiment and of the additional educational analysis of titrations, not only for the adjustments, but also to guide and interpret the discussions. The results in the workshops were that participants could reach consensus on values of n after discussing the unexpected results of the acid-base titration of the unknown 'Pelouze's acid' (maleic

acid) with the indicators methyl orange and phenolphthalein (Van Hoeve-Brouwer and De Vos, 1994; Van Hoeve-Brouwer and Velzenboer, 1995).

6.4.2 Considerations on an educational structure

The chemistry content of the educational text consisted of the molecular structure theory. This theory was used as a result of the educational analysis of chemical bonding reported in Chapter 2. The design for the educational text was to develop an empirical formula, a molecular formula and a structural formula for two substances in that order, and to attribute various meanings to the dashes in these structural formulae (adding layers of meaning). In Section 5.6.2 I could describe the sequential contingency of the structural formulae by using correspondence terms such as a sequence of mass context, mass + distance context and mass + distance + charge context.

By recognizing these contexts in the episodes of the narrative for the educational text and by recognizing these contexts in successive meanings of representations of the structural formulae and the dashes, I could adjust the educational text for the second experiment. It was expected that this would enable students to recognize these meanings in the various contexts. Although I can describe what the students were saying and drawing in the trial with the hydrogen bond in terms of 'belonging together', 'having another position' and a 'certain attraction', I think it is too early to describe their learning in terms of the mass, distance and charge contexts or of switching or combining these contexts. In this case, however, the sequence in the reasoning of the students working in the Lewis episode was first 'belonging together', then 'having another position' followed by a 'certain attraction'. The charge context had been attributed to this episode and, furthermore, it was stated in Section 5.6.2 that each subsequent context would include the previous ones. The students in the trial with the hydrogen bond seemed to pass through the subsequent contexts *within* the charge context during their discussions. *I see this as significant for the educational structure in a mass-distance-charge sequence in this process of learning chemical bonding, i.e. a covalent bond in the framework of the molecular structure theory.*

The remarks made about the 'creation of knowledge' results also apply here. More investigations need to be carried out to see whether it is possible to draw more general conclusions from experiments with the sequence of contexts. In this case the questions are: can similar results be found in other groups with the same teacher, or with other teachers and in other schools? Can similar results be found in lower grades, where students encounter concepts relating to chemical bonding for the first time? What will be the results when the educational text 'Kennis Maken' is used in another school system, for instance, in another country.

If the same assumption as that behind teaching chemical bonding on the basis of the molecular structure theory (sequential contingency) and the same objective of creating knowledge (as the global context) are considered applicable in these new situations, it is

necessary to be very explicit about the concepts and procedures which must be dealt with prior to introducing the educational text 'Kennis Maken'.

Although the educational experiment reported in this thesis took place in the period just before the final exams, the educational text can be adapted to be used as an introduction to the molecular structure theory in an earlier stage. An proposal for such a text is given in the next section.

6.4.3 *An introduction to the molecular structure theory*

This subsection describes a draft for an educational text designed to *introduce* the molecular structure theory to secondary school students. Students are supposed to attach meaning to some chemical concepts, such as the element concept, stoichiometry, valencies, acids and bases, atoms and molecules, molecular formulae and some simple structural formulae, and preferably they should have some experience with titration.

The design of the text is based on the tentative educational structure mentioned above, i.e. mass context, mass + distance context, and mass + distance + charge context.

A. Mass context

1. Provide students with a white powder (malic acid) and a description of some of its properties (melting point, acid, ...). Call it 'apple acid'; formula $C_4H_6O_5$. Study some of its properties in the laboratory (verification of the information provided).
2. Students heat some apple acid gently in a test tube. Crystals appear halfway up the tube. Question: do we call this apple acid or is it something else? Provide students with some maleic acid (second substance) and tell them to compare the two samples and answer the question. Agree on a name for the new substance.
3. Verify C and H in the second substance in separate experiments by heating with an excess of CuO, using either lime water or anhydrous copper sulphate.
4. Refer to Pelouze, 1834. Show authentic descriptions. Tell students that P found a second reaction product at the bottom of the tube. Agree on a name. P was able to determine percentages of C and H in both reaction products. Give data obtained by Pelouze. Discuss the role of oxygen. Let students find the empirical formula CHO. Speculate about n in $(CHO)_n$.
5. Students dissolve 200 mg of maleic acid (use the name given by the students) in water and titrate with methyl orange and 0.1 M NaOH. They interpret the results in terms of amounts of hydrogen. Result: $n = 4$ or a multiple of 4. Second titration using phenolphthalein as the indicator. Results are interpreted in terms of dibasicity of the acid.

B. Mass + distance context.

6. Students use ball-and-stick models to hypothesize with possible structural formulae. Class results are shared. Possible structures of 'apple acid' and its dehydration products are included in the investigations. Rotation around C=C raises questions about substances. Refer to Van 't Hoff.
7. Students are confronted with a substance $C_4H_2O_3$, obtained by dehydrating the first reaction product. The second reaction product does not show dehydration. Speculations about *cis-trans* isomerism. Ball-and-stick models provide answers

with different structures. Introduction of 'real' names: maleic acid (*cis*), fumaric acid (*trans*), maleic anhydride.

8. Addition reactions at C=C bond: water, hydrogen, bromine. Network of organic substances. Then a description of a reaction product obtained from MA and styrene (Wagner-Jauregg) is given. Polymerization as a special case of addition. Use of polymers in society.

C. Mass + distance + charge context

9. Valencies interpreted in Lewis terms, using octet (and, in the case of H, 'duet') rule. Simple model of the atom: some electrons in the periphery of Rutherford's atom are valency electrons. Noble gas configuration becomes criterion for stability. Tetrahedron shape of C (and O). New meaning of dashes. Introduction of electron density and electron density figures.

10. H bonds are introduced, first in water, explaining its unusual behaviour compared with H₂S, NH₃. Description in terms of delta plus and delta minus, attributed to apparent shift in position of the bonding electron pair in O-H bonds. Then H bonds in maleic acid (intramolecular) and fumaric acid (intermolecular), explaining differences in solubility and melting point. Main theme: molecules are not isolated, as the structural formula seems to suggest.

This design can be continued with other concepts and procedures depending on in what depth the molecular structure theory is to be introduced at that point in the school curriculum.

The approach includes several occasions for students to 'create knowledge', but they also learn 'canonical' chemical knowledge. The sequence of concepts introduced is based on the sequential contingency as given in the educational experiment of 'Kennis Maken', but adapted to suit an earlier stage in students' school career. One adaptation is, for instance, the use of ball-and-stick models to generate a hypothesis on the carboxylic groups (cf. Section 3.3.1). The emphasis is on starting from the substance and on the use of structural formulae as models. Of course, the approach needs further research before it can be worked out more fully and be implemented on any large scale.

6.4.4 A teaching structure on the basis of reactions

Within the same assumptions with regard to the tentative educational structure of chemical bonding, another sequence of contexts could be designed when the guiding principle of starting from the substance is replaced by starting from the reactions.

The choice of starting from the reactions as guiding principle can be seen in the educational text "Chemie in Duizend Vragen" developed by De Vos for an introduction into chemistry (De Vos, 1995. An English version entitled "Chemistry in a Thousand Questions" is available).

The students' first encounter with the phenomenon of reactions is when they grind two substances together in a mortar and discuss the results (cf. De Vos and Verdonk, 1985a). The next series of reactions is to be performed in a petri dish which makes it possible to show reactions in a spatial sense by observing the movement of substances,

(cf. De Vos and Verdonk, 1985b). In my interpretation, *starting from reactions needs a corpuscular visualisation in a design in which the distance context is dealt with before the mass context.*

A preliminary sequential contingency could be established as follows, by answering the question: Which reaction characteristics are attributed to which representation and in which context (expressed in correspondence terms):

	<i>Reaction as</i>	<i>Particle</i>	<i>Context</i>
1	(phenomenon)	(macroscopic)	(distance/time)
2	rearrangement of elements	elements as mass portions (non-corpuscular)	mass
3	rearrangement of atoms	atoms as mass portions (corpuscular)	mass
4	rearrangement of charges	ions	charge
5	rearrangement of bonds	atoms in molecules	energy (?)

I draw attention to three differences between the sequence of contexts in this overview and in the sequential contingency as described in the previous sections.

First, as I have already mentioned, the distance context seems to precede the others. This is, perhaps, implicit in the description of a reaction as 'a rearrangement'. However, this idea makes it possible to give an interpretation of distance in a spatial sense to a remark by Pelouze on the various arrangements of groups to explain isomerism (cf. Section 5.3.1). Secondly, starting from reactions might be regarded as a process-oriented approach rather than the static approach of starting from the substances. Consequently, time as a correspondence term is present in the model aspects of the process. Therefore the first context is a combined distance - time context. Thirdly, in this overview, the rearrangement of bonds could be regarded as belonging an energy context, since stability will be a decisive factor on which substances are produced. The energy in this context is to be seen as chemical energy (cf. De Vos, Van Berkel and Verdonk, 1994).

I would like to make two more remarks with regard to this overview, (i) on the occurrence of ions as corpuscles and (ii) on the meaning of valency in the subsequent descriptions of a reaction.

(i) If reactions are to be described in terms of ions, the two-step thesis of the acceptance and use of models may be regarded as applicable for the ions as corpuscles.

As I argued in Section 2.1, the introduction of the free atom in a physics context does not allow for the introduction of ions except for those of low positive charges. Therefore, if ions are to be included in descriptions of reactions and substances, ways must be found of introducing the negative and complex ions. In my view, the acceptance of ions might call for a different interpretation of the corpuscular hypothesis than that which is applicable for atoms in molecules. If this is so, it could explain why electron affinity is a useful concept for the ion model and ionic bond. Furthermore, the difficulties

of introducing the role of electronegativity when combining ionic bonds and covalent bonds can be interpreted as being related to combining models which belong to two different contexts.

(ii) In the discussion of the titration assignment in Section 5.5.2 I included the feature of counting, i.e., counting masses, charges and dashes. These counting activities can now be described as counting of valencies. This counting can be added to the overview of reaction rearrangements mentioned above. The different kinds of valency are: (equi)valent (2 and 3), electrovalent (4) and covalent (5). The first, (equi)valent, can be regarded in the element (non-corpuscular) sense as number of mass portions and in the model (micro) sense as a number of corpuscles. Difficulties will arise when the 'valency values' are not whole numbers, as is the case when partial positive and negative charges are used in the hydrogen bond or polar atomic bond representations. Then, the continuous charge distribution clashes with the discontinuous character assumed for the corpuscles.

An extensive educational analysis could reveal whether, and if so, how, various types of bond can be introduced together. As result of my research, I am inclined to regard this as only feasible in conjunction with the idea of the relativity of models.

6.4.5 Introduction of a new educational text

When an educational text showed to be valuable in a research project the question remains whether the text or other results of the research project can be relevant for introduction in the regular school practice. As an example, I discuss three categories of requirements and consequences which should be taken into account when introducing new educational material such as 'Kennis Maken': requirements for the implementation in the classroom, the required knowledge and skills asked of the teachers, and the possibility of applying the recontextualization guidelines for writing of schoolbooks. Insights from education developmental research should be taken into account with regard to introducing new texts.

The comparison of education developmental research and concept developmental research indicates similarities such as the function of an educational text in both conceptions of research. However, a dissimilarity is the subsequent use of the educational text. In education developmental research, texts are developed for use in the school practice, and in the developmental work, the aspects of implementation, teachers' education, counseling, test development and opinion shaping have already been considered (Gravemeijer, 1994b, p.108).

In concept developmental research, the texts are designed primarily for the purpose of researching concept development and not intended for large scale implementation. When the texts are considered of value for use in schools, measures as mentioned above for education developmental research should be taken into account for any large scale implementation.

Implementation of a text such as 'Kennis Maken' entails taking account of the regulated openness of the text. This means, for instance, finding ways to assess the 'open' assignments. Furthermore, time and space must be available for small group discussions. The method of working in a small group allows the students to work independently and at their own pace, but it requires a considerable degree of flexibility in the school organization, and new skills of teachers to teach according to this method of working.

These requirements indicate the importance of further training for teachers to cover both the chemical content of this new educational material and how to teach it. The creativity of the students may have implications as to the chemical knowledge required of the teacher. To assess the validity of the students' unforeseen arguments, teachers will need more extensive knowledge. During the development of the educational text 'Kennis Maken', several in-service courses were given for teachers. These courses proved to be valuable for both teachers and educational researchers. Working together on the ideas and objectives of the educational text was essential to provide common ground for discussing and making decisions on the design. Teachers who consented to experiment with the educational text benefitted from the discussions during the course when using the text in their classes. A more comprehensive approach to teacher education in combination with development of educational material can be found in the work of Acampo and De Jong (1994)

The last requirements I want to discuss concerns the usefulness of the recontextualization guidelines for the writing of school books. School books will become more and more important because of the Dutch Government plans for reforming advanced level education. According to these plans the teachers' role will change from ex cathedra lecturing to guiding the students' learning processes. Students are expected to study more independently and organize their own learning. The plans for reforming advanced level education include the design of a new exam syllabus. This will require new textbooks. An important problem is that a new approach to teaching (and learning) calls for a new approach to designing textbooks. Course books already occupy an important place in contemporary school practice, and this will become even more so if the new plans for reform are implemented. *The changing role of the teacher will result in a 'teaching through texts'*. Students and teachers will become more and more dependent on how the chemical concepts and procedures are presented in textbooks. It is therefore essential that these new educational texts to be developed should be of the highest possible quality. This implies carrying out educational research including experiments with 'crude' texts in classrooms. An educational structure should provide for concepts and how they are related to each other (e.g. sequential contingency), and the global context and its effect on the meaning of the chemical concepts should also be taken in consideration.

When I consider the work reported in this thesis from the point of view of concept developmental research the result is a tentative educational structure for molecular chemical bonding in terms of mass, distance and charge contexts. Further concept developmental research could extend this educational structure to include time and energy, and other possible sequences than those described in this thesis. The tentative educational structure can be derived from and reinforce the sequential contingency of the educational text. In this way, education developmental research can benefit from concept developmental research.

When I consider the work reported on in this thesis from the education developmental research point of view, I suggest that the implementation of texts designed for concept developmental research should be advanced by applying the methods of education developmental research.

The objective of bridging the gap resulted in the idea of teaching the relativeness of models. This idea led to the development of the global context of creating knowledge as a human endeavour. The guiding principle for the educational text was inspired by the example of chemists working with substances, leading to teaching structures in chemistry.

Epilogue

Looking back on the research project and the report, I can now make some comments of a more general nature.

My personal reason for doing the research project was a teaching problem that I had encountered as a teacher and as a member of the *Gebruikersredactie*. The problem was associated with the teaching of atomic structure in relation to chemical bonding in upper secondary school classes. Participating in the research programme of the Department of Chemical Education implied that both concept development issues and education development issues associated with this topic could be addressed.

As far as atomic structure is concerned, the project has resulted in

- (i) an improved introduction of a simple distance and energy model of the atom within the framework of the existing curriculum;
- (ii) after further analysis, a rejection of atomic structure as an appropriate starting point for teaching chemical bonding. Atomic structure is an unsuitable basis for teaching chemical bonding in secondary schools because there is a gap between the models of free and bonded atoms that cannot be bridged.

Consequently, choosing another starting point solves the original teaching problem. This is a significant result in the framework of education developmental research.

As for chemical bonding, a new question has emerged, *viz.* how this topic can be introduced now that the introduction on the basis of atomic structure has been rejected. An alternative was found in teaching the *molecular structure theory* with emphasis on creating knowledge and using models. Key concepts in this introduction are chemistry, substance and structural formula. An introduction along these lines offers opportunities for concept developmental as well as education developmental research.

The twin pair of maleic acid and fumaric acid were selected as examples to illustrate various chemical concepts throughout the text. This decision, which was to some extent intuitive, shows the following advantages:

1. It offers a framework within which students can interpret new knowledge and link it to things they already are acquainted with.
2. Choosing two related substances rather than one substance creates several possibilities for comparison, thereby convincing students of the need to represent both differences (i.e. anhydride formation) and similarities (i.e. chemical composition) in the structural formulae.
3. There are several experiments on chemical and physical aspects of maleic and fumaric acids suitable for a school laboratory.
4. There are important links with modern chemical technology and societal issues.
5. There is a wealth of relevant historical documentation on these acids offering possibilities for illustrating the creation of knowledge and the use of models.

6. Maleic acid and fumaric acid are associated with several important aspects of the molecular structure theory. These aspects include: the sequence of empirical formula - molecular formula - structural formula; functional groups (COOH and C=C); ordinary and cis/trans isomerism; mutual influence of functional groups; intra- and intermolecular hydrogen bridge formation; and various types of polymerization reactions.

The format of a narrative, i.e. 'biography', allows for an educational structure in which mass, space (distance) and charge are subsequently developed in a stepwise process as dimensions of chemical formulae that represent chemical and physical properties of a substance. Further research could explore the charge context with electrostatic energy notions to develop the energy dimension. Energy would involve heat movement as kinetic energy and electrostatic (Coulomb) energy as potential energy. The time dimension could also be introduced by including reactions as processes, thereby covering kinetics and reaction mechanisms.

In the biography of the substances, information from various sources was incorporated without pursuing to teach the history of chemistry. The search for relevant articles in the framework of a fluid enquiry in the global context of making knowledge led me to look for early publications and go back in history, because knowledge is a continuous stream and because it would enable me to start from the substances, i.e. closer to the relation between experiment and theoretical description. Information from articles and books which can be considered as stable enquiry in science, can be recontextualized as fluid in education by designing suitable assignments within the framework of the chosen sequential contingency of the molecular structure theory. Another valuable source of information for educational purposes can be found at conferences where scientists report their findings, or in publications meant for a broader audience than the narrow group of specialists. Depending on the chosen global context, scientific, technological or societal, information can also be gathered in the field at factories, industrial laboratories, food inspection departments, etc.

The educational experiment reported in this thesis could only be held in a pre-university class because the chapter on chemical bonding came at this point in the curriculum. Two consequences deserve attention.

Firstly, staging the educational experiment in the upper secondary level offered the possibility of taking the corpuscular nature of matter as knowledge acquired by the students in earlier years. I could therefore focus on the second step of the thesis of reduction, i.e. the use of corpuscular models. The interpretation of the empirical and molecular formula was built on the assumption that students had accepted the corpuscular hypothesis. In the titration assignment, a transition from molar mass in the non-corpuscular sense to a molecular mass in the corpuscular sense could not be dealt with.

Students' learning difficulties with regard to chemical bonding, also in this stage of their school career, might in some cases be related to an interpretation of empirical and molecular, i.e. molar, formulae in a non-corpuscular way. Further educational analysis of the titration assignment could clarify whether these learning difficulties arise from a failure to integrate the corpuscular hypothesis into students' previous knowledge or from an inadequate presentation of the topic in teaching materials.

Secondly, when designing the educational text, several concepts taught in earlier years were used (cf. the overview in Section 1.1). The research project has yielded suggestions for a well thought-out educational experiment aiming at the introduction of the molecular structure theory in secondary education. In a sense, a gap has to be bridged between elementary chemical education and the molecular structure theory as presented in 'Kennis Maken'. The introduction of the molecular structure theory implies, in that case, that accepting the corpuscular hypothesis has to be explicitly taught. In general, two routes are possible. One is presenting the corpuscular nature of matter as a working hypothesis and gradually developing the idea of molecules as corpuscular models, after initially accepting the conception of molecules as *minima naturalia* (cf. *Chemie in Duizend Vragen*, De Vos, 1995). The other route is a prolonged use of empirical and molar formulae in the non-corpuscular sense, leading eventually to the necessity of using corpuscular models of molecules. (The start of a comparable route in a stoichiometric sense has been explored by Vogelezang, 1990.)

An educational text aiming at teaching ideas originating from further educational analysis of accepting the corpuscular hypothesis might include using the titration experiment to explore the transition from molar mass to molecular mass, combined with a transition from an empirical formula and molar formula in the non-corpuscular sense to an empirical formula and molecular formula in the corpuscular sense. Educational analysis should establish which substances and reactions can be introduced before maleic acid and fumaric acid can enter the stage in their biography, 'Kennis Maken'.

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Appendix: The Educational Text

GETTING ACQUAINTED

or

THE STORY OF A SUBSTANCE

An Experimental Unit Written For The Research Project On

"AN EDUCATIONAL STRUCTURE FOR CHEMICAL BONDING"

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GETTING ACQUAINTED

1. INTRODUCTION

This is the life story of a chemical compound. We shall follow its history from the formation of the first crystals at the beginning of the last century through the gradual progress of scientific research to its applications in industry today. The history of the compound is also the history of people creating knowledge: how they became acquainted with the substance and got to know it better, using the knowledge they already had to investigate it and then using the results of their investigation to formulate theories and investigate other compounds. They made notes of their work to accumulate a growing body of knowledge about the properties of the compound; they discuss the results of their work with each other and pass on new information by writing letters, giving lectures or publishing articles or books.

We are not going to concern ourselves with all aspects of past history. In getting acquainted with the new compound, you will be using a combination of techniques dating from the period when the compound was first identified and other techniques which will depend on the equipment available in your school. You will be learning some new chemistry, but above all you will be learning to find new links between things you already knew. In this way, this programme will help you build up the skills you will need for your Advanced Level work.

The work will be done in groups, because this is the way chemists work, and also because it will give you an opportunity to discuss the work and learn from each other. Some assignments will be divided over a number of groups, each of whom will report their findings to the other groups, who may need this information for their task. This saves time. When writing your reports, don't forget that you have to make your findings clear and understandable to the others as well as to yourselves! At the end of each paragraph, list what you consider to be the main points, and any questions they raised in your mind.

2. PELOUZE

The story starts around 1830 in a French laboratory where people were researching plant and fruit extracts. They were excellent chemists, though most of their experiments look rather old-fashioned to us today. Their aim was to draw up an inventory of organic chemicals describing the properties and reactivity of as many compounds as possible. They dissolved and heated these compounds, made precipitates and recrystallised from solutions, etc. etc. One of these compounds was malic acid, a white powder which the chemists of the age could isolate from apples. In a German publication in 1834, the Frenchman Théophile J. Pelouze reported the following about his experiments:

"After these experiments I started dry distillation in an oil bath; with a thermometer the temperature could be observed accurately. (...) The colourless liquid could be seen rising up the sides, and soon the liquid changed into beautiful prismatic crystals. (...) When starting with 10 grams, the transformation is completed in two hours."

Experiment 1 Heating malic acid

Carry out the dry distillation of malic acid in a fume cupboard as follows:

Place a small amount of malic acid in a tempered glass test tube.

Heat the tube with a small colourless flame until the malic acid has been converted.

Compare your results with those of Pelouze.

Keep the test tube and its contents for experiments 2 and 3.

Later in the same article, Pelouze describes a number of properties of the chemical he found on the sides of his flask:

"It has no smell, it tastes acidic initially, but with a very unpleasant aftertaste. It dissolves easily in water and in alcohol; these solutions colour litmus red. The solution in water does not precipitate with lime water. With barite water it produces a white precipitate in the form of small, glossy flakes."

Experiment 2 Properties

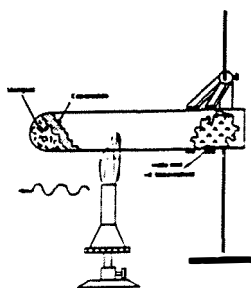
Check these properties (except for the taste) on the contents of the test tube you used in experiment 1, and see if you can add anything to the description.

Remember that you are working with an unknown chemical and you have no safety instructions to guide you! Discuss your ideas for experiments with your teacher before you carry them out.

Report your results to the other groups.

Experiment 3 Qualitative element analysis

Pelouze assumed that the white substance was a simple organic acid. You can verify whether the compound so formed contains carbon and hydrogen with the following experiment:



Mix a little of your own chemical product with about 5 times as much copper oxide powder. Put this mixture in a dry test tube and top it with a layer of copper oxide.

Clamp the test tube almost horizontally to a stand and seal off the tube with cotton wool sprinkled with a little dehydrated copper sulphate. Have a test tube with clear lime water ready.

Heat with a powerful flame, first under the centre of the test tube to heat the pure copper oxide, and then when that changes colour, move the burner so as to heat the compound at the bottom of the tube.

Note the colour of the copper sulphate in the cotton wool.

Pass the gas which is given off through the lime water and observe whether it becomes cloudy.

Report your conclusions and show how you arrived at them.

Around 1830, Liebig (one of Pelouze's teachers) developed a method for carrying out similar experiments *quantitatively*. Pelouze therefore knew how to work out the empirical formula of a chemical compound. He assumed that the acid he was investigating, which we shall call 'Pelouze's acid' for the time being, contained only oxygen in addition to carbon and hydrogen.

These are the results of Pelouze's quantitative analyses as published in his article:

	I	II	III
Carbon	41.30	41.32	41.31
Hydrogen	3.46	3.44	3.60
Oxygen	55.24	55.24	55.00
These analyses indicate the following composition:			
1 At. C	76.438		41.84
1 - H	6.239		3.41
1 - O	<u>100.00</u>		<u>54.75</u>
	182.677		100

Assignment 1

- How do you think Pelouze calculated the proportion of oxygen?
- Calculate the empirical formula of Pelouze's acid with the data from the chart and the values for atomic masses generally accepted today. ¹

In his article, Pelouze reported the formation of not one but *two* new compounds when he heated malic acid in an oil bath. He described the second substance, which he found in the bottom of the flask, as follows:

"About 200 parts of water are needed to dissolve this substance whereas the other chemical dissolved in an equivalent weight of water; the taste is purely acidic; it crystallises into heaps of narrow pillars the shape of which is difficult to determine (...) It does not melt readily when heated, and does not evaporate until it reaches a temperature of over 200°C. (...) The acid in solution gives no precipitation with lime water or barite water."

The qualitative analysis of this compound yields almost the same results as for Pelouze's acid. Therefore, the other compound formerly known as 'moss acid' must have the same empirical formula.

Assignment 2

- Collect all the data you can find in the above on the properties of 'moss acid', Pelouze's acid and your own product from experiment 1, and make a summary. If more data are available for some compounds than for others, try to find the missing properties of the others by carrying out more experiments, after consulting your teacher.
- What similarities and what differences can you find?
- What conclusions can you draw?

The next step in examining a chemical compound is to draw up a molecular formula. This formula may be the same as the empirical formula, or a multiple of it. To determine this formula, we need to know the molecular mass. We can find out more about the molecular mass by titrating a measured amount of acid with a sodium hydroxide solution. Strangely enough, you do not have to titrate very accurately: you just

¹ In Pelouze's days, these values for atomic mass had not yet been accepted by all chemists, and consequently, different formulas were sometimes in use for the same compound. We shall disregard this problem here.

need to determine a simple whole number in order to derive the molecular formula from the empirical formula. But when you do not know whether an acid is strong or weak it is difficult to choose a suitable indicator. We shall take two indicators, phenolphthalein and methyl orange, which change colour in two different pH ranges.

Experiment 4 Titration of Pelouze's acid

Two titrations will be carried out with Pelouze's acid, the first with phenolphthalein as an indicator and the second with methyl orange.

Weigh 200 mg of acid on a scale.

Add 10 ml of distilled water.

Add 5 drops of indicator solution

Titrate with 0.1 M NaOH until the indicator has changed colour.

Calculate for each experiment how many moles of H^+ have reacted.

Collect the results from all the groups and try to work out the molecular formula.

Experiment 5 Titration of 'moss acid'

Once again, two titrations will be carried out, one with phenolphthalein and one with methyl orange as the indicator.

Weigh 200 mg of acid on a scale.

Add at least 5 ml of alcohol to accelerate the dissolution process; shake carefully for a few minutes.

Add 10 ml of distilled water.

Add 5 drops of indicator solution

Titrate with 0.1 M NaOH until the indicator has changed colour.

Calculate for each experiment how many moles of H^+ have reacted.

Collect the results from all the groups and try to work out the molecular formula.

The results of the titrations may have confused you at first. There is no way you can be sure whether the answers are right or wrong. That's the way it is with scientific research: you do not know the answers before you do your experiments, though you usually have a general idea of what kind of answers to expect. You may well be making new observations, which you have to try and fit into the framework of existing knowledge.

The terms 'valence' and 'structural formula' did not have the same meaning for Pelouze as they have today, although even in his time symbols were arranged in groups in a formula, such as the group we call the carboxylic acid group today.

Assignment 3

Using the molecular formula of the acids, write out all the structural formulas that correspond with the valences as we know them today and with the data you found on the properties of the acids.

Fortunately, there are not many possible formulas, and you will probably be able to decide together which ones to rule out and which to retain. The structures show that the compounds are acids, and they will probably indicate whether there is a double bond between the two carbon atoms. This is a hypothesis we can test.

Experiment 6 Reaction with bromine water in darkness and light

Weigh 2 grams of Pelouze's acid and shake this with 20 ml of distilled water.

Add 5 ml of bromine water and divide the mixture over two test tubes.

Put one tube away in the dark and leave the other one on the bench.

What do you observe?

Pelouze and his coworkers drew up a molecular formula for both acids. They named Pelouze's acid *maleic acid* ('acide maléique'), indicating that the compound is chemically related to malic acid, ('acide malique' in French).

The naming of chemicals was just as problematic then as it is today. In most cases the name was based on the fruit or plant from which it was isolated. If a compound could be extracted from more than one source, it was sometimes known under different names, according to the source. Once it became clear that these names referred to one and the same compound, one of these names had to be chosen as the official name to be used from then on. This is what happened in the case of 'moss acid', a compound that can be isolated from certain types of moss. It turned out to be identical to fumaric acid, a compound that could be extracted from *Fumaria officinalis* or common fumitory. We also know that this chemical is identical to the second product derived from heating malic acid. The name that was chosen in this case was *fumaric acid*.

Assignment 4

How can you establish that you are dealing with one and the same chemical compound?

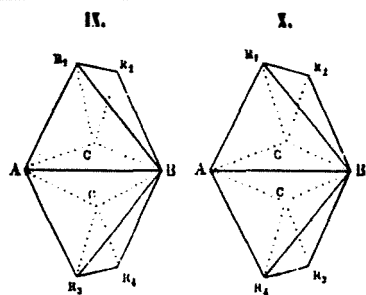
This chapter becomes the story of *two* compounds, fumaric acid and maleic acid. Both are white and crystalline, they have both similar and dissimilar properties, they have the same molecular formula: a pair of isomers.

So we know quite a lot about these compounds already, but there are more questions we can ask, such as: what are the structural formulas of maleic acid and fumaric acid?

3. VAN 'T HOFF

To find an answer to this question, we have to leap in time from 1832 to 1874. This part of the story takes place in a study in Utrecht, the Netherlands, where Johannes H. van 't Hoff decided to publish his ideas about how to represent carbon atoms in a pamphlet entitled "Proposal for the extension of the structural formulas currently used in chemistry today to include a spatial dimension". He writes amongst other things about compounds with a double bond between two carbon atoms:

"A double bond can then be represented by two tetrahedrons joining along one edge (Fig. IX). A and B indicate the bonds between the two carbon atoms, and R1, R2, R3 and R4 the univalent groups. This way, the remaining affinities of the carbon atoms are satisfied."



"The differences between these figures, of which there are two, predict isomerism.

It was not possible to show this with the original system of representation."

A carbon atom with four possibilities for bonding will look like a tetrahedron. With a double bond there will be two of these tetrahedrons with one edge joining. If you imagine different groups on the other corners of these blocks, there will be two possibilities: R1 and R2 opposite R3 and R4, or R1 and R2 opposite R4 and R3 respectively. If both carbon atoms are carrying an H and a COOH, there are two possibilities: H opposite H and COOH opposite COOH or twice H opposite twice COOH. Van 't Hoff thought that this could explain the isomerism of maleic acid and fumaric acid.

"These acids are in fact as described above: *Two double bonded carbon atoms each carry two different univalent groups, H and COOH.*"

In his "Proposal" Van 't Hoff shows with examples that structural formulas can be depicted three-dimensionally. This was a completely new idea at that time. Although one might expect this new idea to be embraced with enthusiasm, the comments of Kolbe, a famous German chemist and contemporary of Van 't Hoff, show that this was certainly not the case.

"A certain Dr J.H. van 't Hoff of the Veterinary School in Utrecht, the Netherlands, appears to have an aversion to exact chemical research. He thought it more appropriate to clamber on to Pegasus' back (borrowed from the Veterinary School no doubt) and declare in his "Chemistry in Space" how, during his brave flight to the top of the chemical Parnassus, the atoms manifested themselves as if they were grouped in space."

Experiment 7 Folding tetrahedrons

The tetrahedron models that demonstrate that there are two possible structures with a double bond can be folded from paper. You need two strips of thick paper, each 27 cm long and 3.5 cm wide.

Fold one strip so that 12 equilateral triangles are formed.

Number the triangular planes 1 to 12 (see A).

Fold the strip so that fold a1a2 lies along fold a5a6 to form a tetrahedron (see B).

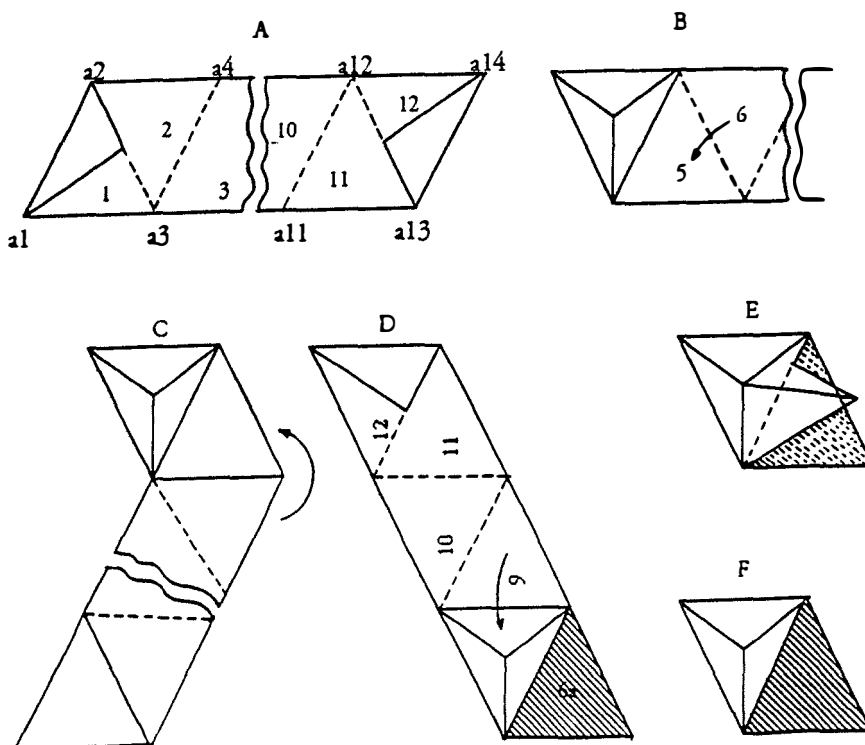
Fold plane 6 over plane 5 and then fold plane 7 against the other side of plane 5 (see B and C) to form a triangular flap or tab which you can use to join the two tetrahedrons later.

Wrap the rest of the strip around the tetrahedron (see D).

Fasten the strip by inserting plane 12 between the lines a1a2 and a5a6 (see E and F).

Fold the second strip of paper in the same way.

Use the projecting triangular tabs to slot the two tetrahedrons together.



The models you have folded look like the tetrahedrons Van 't Hoff made. According to Van 't Hoff, this method of representing a double bond made it possible to explain a certain type of isomerism, which we call *cis-trans* isomerism today. Different structures belong to different compounds. With *cis-trans* isomerism, there is a fixed bond with fixed positions for certain groups, which is not the case with a single bond. These bonds rotate easily around the axis of the single C-C bond. Because of this flexibility, the groups can shift their positions so that one configuration becomes another, and there is no question of isomerism. Butanedioic acid, for example, shows no *cis-trans* isomerism.

We have two chemical compounds, maleic acid and fumaric acid, and there are two structural formulas, *cis* and *trans*: which compound has which formula? We can again use the results of Pelouze's experiments. He found that by heating maleic acid further, water is released and a new carbon compound is produced. Fumaric acid does not react like this when heated. To establish that a new compound had been formed from maleic acid, he determined the composition of the reaction product. He gives the following mass percentages after two experiments:

Carbon	48.67	48.78
Hydrogen	2.17	2.10
Oxygen	<u>49.06</u>	<u>49.12</u>
	100	100

Assignment 5

Calculate the molecular formula of 'water-free maleic acid' using Pelouze's results, and draw up a structural formula.

Does this structural formula help you to choose which structural formula belongs to maleic acid? Explain your answer.

No experiments will be carried out with 'water-free maleic acid' (now called maleic acid anhydride) because this compound can only be handled with great care. We shall use experimental data to check the answer. Van 't Hoff reached his conclusion by using the difference in the degree of acidity, as described in the book he wrote in 1899. As a measure of the degree of acidity he used the "first ionisation constant". The constant for maleic acid is 1.17 and for fumaric acid 0.093. He records as well that the acid salt of maleic acid is a weaker acid than the acid salt of fumaric acid.

Assignment 6

- Explain what is meant by "the ionisation constant of maleic acid is 1.17", using a chemical reaction equation if necessary.
- How can the ionisation constant be used as a measure of the degree of acidity?
- Which structural formula and which name can you give to the "acid salt" of maleic acid?

Assignment 7

With the aid of structural formulas you can predict how different groups will influence each other.

- Use this to try and work out an explanation for the difference in the degree of acidity of maleic acid and fumaric acid.
- Examine whether this can also be used to explain the difference in the degree of acidity of the acid salts of both acids.

In organic chemistry, chemists use structural formulas to communicate with each other about chemical compounds. This is a clearer way of exchanging information than by referring to the compounds by name, even though the nomenclature is based on the structural formulas.

A chemist can derive a great deal of information from the structural formulas about the reaction possibilities and other properties of the compound. In the next section we shall find out how further knowledge was built up about the relationship between the structure and the properties of a compound.

4. LEWIS

In 1923, Gilbert N. Lewis, a professor at the University of California, published a book in which he sets out the structural formulas of maleic acid and fumaric acid in the *cis* and *trans* form, observing that:

"Here the number of atoms separating the two carboxyl groups is the same in both acids, and we might therefore expect that the dissociation constants would be very nearly the same."

Lewis argues that in organic chemistry each characteristic group (eg. -COOH or -OH) represents a set of properties (acid, capable of being oxidised) and that all properties of a

compound are the sum of these sets of properties. But the structural formulas sometimes indicate that the different groups can influence each other. Take oxalic acid for example: the second step of ionisation is weaker than the first. This is explained by the electrostatic interaction between a -COO^- and a -COOH group. Lewis assumed that when comparing fumaric acid and maleic acid, properties, such as acidity, can be predicted more precisely by taking into account the *distance* between certain groups within the structure. There are two acids, each with two carboxyl groups and these should be equal in strength because in both cases there are two C atoms between the acid groups. However, he records the same difference in acid strength as Van 't Hoff, and he writes:

"It seems evident that there is an opportunity for a spatial approach of the two carboxyls in the one case which is absent in the other, and that this approach enormously heightens the mutual influence of the two groups."

The two quotations are from the section of the book where Lewis is trying to establish a connection between the possibility of certain reactions and the displacement of electrons. He elaborates his theories in his book "Valence and the Structure of Atoms and Molecules".

The atom is seen as a nucleus surrounded by electrons that are distributed over shells. Lewis called the electrons in the outer shell of the atom the valence electrons. Two atoms are held together by the valence electrons, which are shared by the two atoms. Helium and other noble gasses have specific chemical properties. Therefore, the valence electron numbers of two and eight are important, according to Lewis. The grouping of valence electrons in sets of eight, later called octets in the "octet rule", is still used today to arrange electrons. Compare for example the number of valence electrons of a sodium ion and a fluoride ion, and you will see that it is the same as for the neon atom: eight.

Lewis argues that it is very significant that all the compounds he investigated had an even number of electrons per molecule. He linked this with the number of electrons of the helium atom and arrived at the *rule of two*, which is that electrons tend to form pairs, both in the atom itself and between atoms.

"The electron pair, especially when it is held conjointly by two atoms and thus constitutes the chemical bond, is the essential element in chemical structure."

Assignment 8

- How many valence electrons does a carbon atom have? And an oxygen atom?
- Draw the structural formula of fumaric acid using lines, and then draw it again with the valence electrons represented as dots.
- Check whether the number of electrons is the same as in a).

The lines drawn between atoms in a structural formula may represent a shared or *bonding* pair of electrons. A pair of electrons belonging to one atom can also be represented by a line. This is called a *lone* electron pair.

We draw a double line to represent a double bond; this means that there are two bonding pairs of electrons. A property of chemical compounds with a double bond in the structural formula is that they are capable of an addition reaction. The two lines in the structural formula depict this possibility. Compare this with Experiment 6.

A conjugated system of double bonds is a special case. Here the structural formula has a double bond followed by a single bond followed by a double bond and so on in alter-

nating succession. To explain certain reactions one has to assume that in a conjugated system the single bond is a little bit 'double' and a double bond is a little bit 'single'². In some reactions it looks as if the double bond can 'jump'.

Assignment 9

When 1,3-butadiene $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$ reacts with bromine you get 1,2-dibromo-3-butane, but also 1,4-dibromo-2-butane.

- Represent these compounds in structural formulas with the electron pairs shown as lines.
- Do the same again, but with the electron pairs represented as dots.

In many countries, Lewis' bond theory is the cornerstone of textbook teaching of chemical bonds, but its limitations are not always made clear. Lewis shows in his book that his theory does not apply in all cases. For example, there are molecules with odd numbers of electrons, and there are also compounds where a deca rule applies instead of the octet rule.

He also demonstrates that some reactions can be explained if it is assumed that the bond electron pair originates from one atom, which he takes to be a lone electron pair. You will find an example in the following assignment.

Assignment 10

- Draw the structural formula of ammonia with all valence electrons in pairs (the Lewis dot diagram).
- Show by means of structural formulas how an ammonium ion can be formed from ammonia in an acid-base reaction.

Lewis believes that the most important addition to his ideas is the hydrogen bond. He puts forward a theory that a hydrogen atom is bound to two pairs of electrons from two different atoms, thus forming a loose bond between these two atoms.

Assignment 11

- Draw two water molecules with the bonding pairs and the lone electron pairs.
- Show where a hydrogen bond is possible between these two molecules.

These loose hydrogen bonds could also explain the difference in acid strength between fumaric acid and maleic acid, not only when comparing the two acids but also when comparing the difference in acid strength between the carboxylic acid groups within the acids themselves. Lewis never applied the hydrogen bond theory in this context.

Assignment 12

- Demonstrate the possibility of hydrogen bond formation within the maleic acid molecule.
What effect do you think this would have on the dissociation of the other hydrogen atom as an ion?
- Show where a hydrogen bond could be formed in the hydrogen maleate ion.

² The benzene molecule could be explained as an extreme case of a conjugated system.

What effect would you expect this to have on the dissociation of the second "acid" hydrogen atom?

c. Answer the same questions for fumaric acid.

d. Explain the possible differences in acid strength as found in the titration experiments 4 and 5.

In this assignment we have looked at the hydrogen bond inside a molecule. Hydrogen bonds can also occur *between* molecules, and this helps us to explain other properties.

5. YARDLEY

When drawing a structural formula we assume that a molecule is floating freely in space, without any external influence. This may be the case for gas molecules, but a molecule in a crystal is surrounded by similar molecules in close proximity, and it is possible that this influences aspects of the structure, such as bond distances and/or bond angles. The next story is about this influence, and research on crystals.

The action takes place in the Davy-Faraday Laboratory of the Royal Institution in London. In 1925, Kathleen Yardley published from this laboratory an article on her research in which she used X-rays to examine fumaric acid and maleic acid. Her aim was:

"to determine whether the planosymmetry and centrosymmetry usually ascribed to maleic and fumaric acids respectively have any actual existence in the crystalline state."

Planosymmetry and centrosymmetry are the old names for cis- and trans-structures. In other words, she hoped to discover whether the cis- and trans-forms attributed to the acids could be detected in these acids in the crystalline state, in some way or another.

Assignment 13

The old names show that people saw certain symmetries in the structural formulas.

Draw the structural formulas for the two acids, showing the symmetries.

Look out for a mirror plane when drawing the structural formula for maleic acid, and an axis with fumaric acid.

"What is symmetry? The first kind of symmetry that springs to mind is the symmetry of a plane of symmetry. Symmetry can also occur in time and space. Sometimes it is a periodical repetition and sometimes a conversion. It is pleasing and has an aesthetic value."

This quotation comes from a book on crystallography by Escher. It does not deal with the symmetry of structural formulas but the symmetry characteristics of crystals. The shape of crystals has long been used by researchers as an aid to identifying and classifying chemical compounds. Today, crystallography and crystallographic analysis play a vital part in the clarification of structures in a spatial dimension. Crystallographic research can be divided into *geometrical* and *optical* research. *Geometrical* crystallography provided the theory and the formulas of angles and planes of crystals, their cross sections and axes. A model is made of the inside of a crystal, with the atoms placed on the junctions of an imaginary three-dimensional lattice.

In *optical* research, waves are passed through the crystal and the effect, such as refraction phenomena, observed. Experiments with refraction by passing X-rays through crystals were set up to establish refraction patterns, but also proved to be very useful when determining the lattice of a crystal. It is interesting to note that the results explained something about the nature of X-rays as well as something about the structure of the crystals. It was discovered that X-rays are waves and that crystals can be described in terms of angles and the distances between atoms. We can examine the structure of chemicals, and make models of atoms, ions and molecules by measuring the distances between atom nuclei. NaCl was one of the first compounds to be investigated in this way, and research revealed that its crystals were arranged in a regular cubic formation. We assume that sodium and chloride particles are positioned at alternating junctions.

What did Yardley find in 1925? There were problems with fumaric acid, in the first place because it was difficult to make good crystals, and further because it appeared to have two different crystal forms. The research on maleic acid progressed better, but certain observations indicated that maleic acid in crystalline form was asymmetrical, and that would mean that there was no plane of symmetry. However, it could be that the molecules were symmetrical in solution and became distorted during crystallisation. According to Yardley, the high melting point of fumaric acid and its poor solubility could be due to a special combination of the molecules in the crystal.

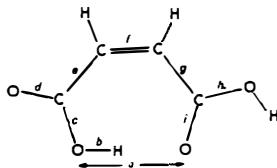
Assignment 14

- Propose an arrangement of fumaric acid molecules in a crystal. Look out for possible interactions between the molecules.
- Try to explain the high melting point (in comparison with that of maleic acid).
- Try also to explain the poor solubility in water.

It takes a lot of calculation to work out the pictures of X-ray diffractions. The advent of computers has opened up wider possibilities in this field. Crystallographers' first interest in fumaric and maleic acid was in seeking to explain the similarities and differences in structure, but today these acids are also used to test certain theories. Hydrogen maleate was and still is the subject of a great deal of research, because of questions about its symmetry and the parity of certain bonds and hydrogen bonds.

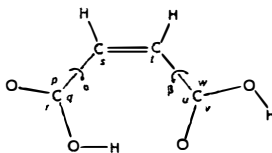
Table 5. A summary of the molecular geometry for maleic acid/maleate ion species

(a) Distances



Compound	a	b	c	d	e	f	g	h	i	Ref.*
Maleic acid	2.502 (1)	0.91 (2)	1.304 (2)	1.218 (2)	1.488 (2)	1.337 (2)	1.475 (2)	1.300 (2)	1.222 (1)	} a
Tricyclic alkene	2.472 (3)	0.78 (5)	1.297 (4)	1.225 (4)	1.492 (3)	1.349 (4)	1.485 (4)	1.300 (3)	1.221 (3)	
Weighted mean	2.512 (3)	1.03 (4)	1.305 (2)	1.219 (2)	1.503 (3)	1.344 (4)	1.487 (2)	1.310 (2)	1.225 (2)	} b
Weighted mean	2.500 (1)	0.92 (2)	1.304 (1)	1.219 (1)	1.492 (1)	1.340 (2)	1.481 (1)	1.304 (1)	1.222 (1)	
Bromphen HMal	2.417 (4)	1.08 (5)	1.292 (6)	1.209 (6)	1.497 (7)	1.329 (7)	1.481 (6)	1.230 (6)	1.265 (6)	b
Chlorphen HMal	2.444 (4)	0.87 (3)	1.280 (4)	1.209 (4)	1.489 (5)	1.331 (5)	1.486 (4)	1.236 (4)	1.266 (4)	c
KHMal	2.437 (4)	1.22 (4)	1.284 (3)	1.235 (3)	1.498 (3)	1.348 (4)	1.498 (3)	1.235 (3)	1.284 (3)	d
KHCIMal	2.411 (3)	1.207 (5)	1.284 (3)	1.230 (2)	1.524 (2)	1.349 (3)	1.512 (2)	1.244 (2)	1.288 (3)	e
cis-Aconitate	2.425 (2)	1.13 (7)	1.291 (2)	1.235 (2)	1.485 (2)	1.345 (2)	1.519 (2)	1.230 (2)	1.287 (2)	f
Weighted mean	2.425 (1)		1.287 (1)	1.230 (1)	1.502 (1)	1.344 (1)	1.509 (1)	1.236 (1)	1.283 (1)	
Na ₂ Mal	3.151 (1)		1.293 (1)	1.281 (1)	1.506 (1)	1.336 (1)	1.495 (1)	1.250 (1)	1.264 (1)	g
Li ₂ Mal	2.999 (2)		1.273 (2)	1.252 (2)	1.505 (3)	1.330 (3)	1.495 (3)	1.252 (2)	1.277 (2)	h

(b) Angles



Compound	p	q	r	s	t	u	v	w	α	β	Ref.*
Maleic acid	119.8 (1)	121.4 (1)	118.9 (1)	131.6 (1)	128.2 (1)	125.1 (1)	122.6 (1)	112.3 (1)	0.0	2.3	
Tricyclic alkene	1 118.8 (3)	121.4 (3)	119.7 (2)	131.1 (3)	127.3 (2)	124.9 (3)	121.4 (3)	113.7 (2)	5.1	4.0	a
	2 119.0 (2)	120.6 (1)	120.4 (1)	130.5 (2)	127.3 (2)	124.2 (1)	122.3 (1)	113.5 (1)	17.7	19.5	
Weighted mean	119.6 (1)	121.0 (1)	119.7 (1)	131.4 (1)	127.9 (1)	124.7 (1)	122.4 (1)	113.0 (1)			
Bromphen HMal	118.6 (5)	119.3 (4)	122.1 (5)	131.0 (5)	130.2 (5)	119.9 (4)	123.2 (5)	116.9 (4)	8.4	6.7	b
Chlorphen HMal	118.8 (4)	120.3 (3)	120.9 (4)	131.5 (3)	129.3 (5)	120.0 (3)	123.4 (3)	116.7 (3)	1.5	7.4	c
KHMal	117.0 (3)	120.3 (3)	122.7 (3)	130.4 (2)	130.4 (2)	120.3 (3)	122.7 (3)	117.0 (3)	0.0	0.0	d
KHClMal	118.6 (2)	118.0 (1)	123.3 (2)	130.6 (1)	129.5 (1)	120.3 (2)	122.7 (2)	117.0 (2)	8.5	9.0	e
cis-Aconitate	117.1 (2)	120.9 (1)	122.0 (2)	132.9 (2)	126.9 (1)	119.6 (1)	121.7 (2)	118.7 (1)	12.5	7.1	f
Weighted mean	117.8 (1)	119.5 (1)	122.5 (1)	131.0 (1)	128.5 (1)	119.8 (1)	122.5 (1)	118.0 (1)			
Na ₂ Mal	113.2 (1)	120.6 (1)	126.1 (1)	129.5 (1)	126.5 (1)	118.6 (1)	125.2 (1)	116.2 (1)	66.3	-16.9	g
Li ₂ Mal	116.8 (2)	119.1 (2)	124.1 (2)	127.4 (2)	125.1 (2)	119.2 (2)	123.5 (2)	117.3 (2)	81.4	7.0	h

* (a) Hechtfischer *et al.* (1970). (b) James & Williams (1971). (c) James & Williams (1974a). (d) Darlow & Cochran (1961). (e) Ellison & Levy (1965). (f) Glusker *et al.* (1972). (g) James & Williams (1974b). (h) Town & Small (1973).

Assignment 15

- Look up the carbon-carbon distances for maleic acid, KHmal and Na₂mal.
- Look up the angles between the carbon bonds for these compounds.
- Can any symmetry be detected?

Assignment 16

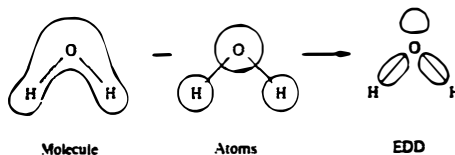
More interesting conclusions can be drawn from the table, particularly for a comparison between different aspects of double bonds.

Compare the distances given in this table for the single and double C-C bond with the values given in your own book of tables.

Are there any indications that there could be any conjugated systems here?

In crystallographic research with X-rays, drawings are made showing the distribution of electron density in a plane or section of a molecule or ion. The electrons are not portrayed as particles, but as a distribution of a negative charge. High and low densities show a high or low charge per volume unit respectively. In the drawings, the points of equal electron densities are connected by a line, just as points with the same altitude are connected up to form contour lines on a map. It is possible to draw maps showing differences in charge using crystallographic measurements and calculations.

For example, in the case of a water molecule the electron density of the single oxygen atom and the two single hydrogen atoms is calculated. Then the electron density of the water molecule is determined with diffraction recordings. The electron densities are subtracted at each point on the two maps. The resulting map shows the changes in the electron density of the molecule due to the formation of bonds. This can be expressed schematically as follows:



Real electron density maps are less clear-cut, and it takes some effort to interpret the various drawings. The following map of maleic acid has been published. The contours show the increments of electron density as compared with single atoms, and the dotted lines indicate the decrease. The drawing shows a section through the mean molecular plane with the atomic nuclei represented by dots.

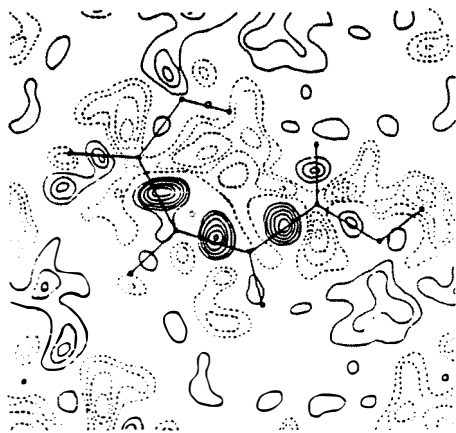


Fig. 5. A section of the final difference electron density map through the mean molecular plane. Contours start at $\pm 0.05 \text{ e } \text{\AA}^{-3}$ and are in equal increments of this value.

Assignment 17

- Are there any indications of the presence of a double bond?
- Compare the results of Assignments 16 and 17a.
- What "reactivity" does this double bond predict for a compound?

Experiment 8 Reaction of maleic acid and bromine solution

A strong light source such as an overhead projector is needed.
 Put a saturated solution of maleic acid in water in a petri dish.
 Add one ml of bromine solution with a pipette.
 Leave the dish for a few minutes in the light.
 Compare your observations with those of Experiment 6.

Research on fumaric acid and maleic acid shows that it is possible to contribute to the solution of theoretical questions. The acid molecules represent simple chemical systems which can be used as the basis for calculations, and the results of these calculations can be compared with the values measured for the acids or related chemical compounds. The properties of other compounds can be understood and predicted with the aid of the knowledge of molecular structures thus obtained. This knowledge about the relationship between the structure and the properties of a chemical, usually referred to as the structure property relation, can be useful in devising new reaction possibilities or inventing new chemicals. These new inventions could be a new medicine, or a synthetic material meeting environmental conditions, or a sweetener that is not too expensive.

6. WORKING WITH CHEMISTRY

It is very difficult to choose a person or a place to continue the story of chemical compounds. All over the world, in laboratories and factories, people are working today on maleic acid, fumaric acid and the related compound maleic acid anhydride. An abundance of information is available: a book containing about ten thousand references to articles, patents and other books has been published on maleic acid anhydride alone.

A lot of the information is connected with the relation between the structure of the molecules and the properties of the chemical compound concerned. This gives chemists an indication of which materials might or might not be useful for certain applications. For example, the sweet taste of a compound is related to a certain spatial distribution of the molecules of that compound. When looking for a new method of synthesising the compound, one has to deal with the fact that several different optical isomers may be formed, whereas only one is suitable.

The following two exercises combine data from different sources and show contemporary applications. The first exercise concerns fumaric acid and the second maleic acid and its anhydride.

EXERCISE I

K. Oyama, a Japanese researcher, describes in his book "Chirality in Industry" a process for producing the sweetener aspartame. This compound is made from L-aspartic acid and the methyl ester of L-phenylalanine.

Assignment

I a. What products might be formed when these two amino acids react with each other?

In every process, the aim is to produce the required product with a minimum of reaction steps while achieving maximum purity. In the case of aspartame, this requires great precision because during the formation of the peptide bond, an isomer of aspartame that tastes not sweet but bitter may also be formed. An enzymatic method has therefore been designed which also allows the manufacturer to produce the product required on an industrial scale, which in this case means thousands of tonnes.

Assignment

I b. What are the advantages of an enzymatic reaction in this case?

I c. What special care has to be taken with enzymatic reactions?

Useful enzymes are isolated from animal organs, plant cells or bacteria. Knowledge of enzymes has a long history, and fumaric acid plays an important part in it, especially with respect to one of the components used in the synthesis of aspartame. We can find data on this in reports on biochemical research of metabolic processes such as the citric acid cycle.

Assignment

I d. Gather information about the position of fumaric acid in the citric acid cycle, for example from a book of tables.

I e. Which differences in structure will be found when malic acid forms according to the citric acid cycle from fumaric acid, as compared with when it is formed with water as in a 'normal' addition reaction?

Explain the differences.

Chemical research is often like a jigsaw puzzle without a picture to guide you, and that was certainly the case when researchers were formulating the citric acid cycle. A contribution to the solution of this puzzle came from research into the equilibrium existing between fumaric acid, ammonia and L-aspartic acid in the presence of resting bacteria.

Assignment

I f. Show by means of structural formulas the reaction between fumaric acid and ammonia by which aspartic acid is formed.

I g. Why could it be useful to introduce a suitable enzyme?

The use of resting bacteria, *E. coli*, was introduced at a time when research into enzymes and their mutual correlation was developing rapidly. One might have expected that by now, a reaction process would have been developed using isolated enzymes to produce L-aspartic acid for the synthesis of aspartame. However, it appeared that although the enzyme can be isolated from *E. coli*, it is not suitable for use in an industrial process. Scientists in Japan discovered that complete cells gave better results. An additional advantage is that these cells can be immobilised. This means that cells can be attached to or built into carrier material.

Assignment

I h. Work out the advantages and disadvantages of a batch process as compared with a continuous process when carrying out a chemical reaction on an industrial scale.

I i. A continuous process is possible with immobilised cells. Show in a diagram how L-aspartic acid could be synthesised from a solution of ammonium fumarate in a continuous process.

Fumaric acid is a component of a chemical compound used to sweeten drinks and foodstuffs. But fumaric acid itself is also a food additive. It may be added to foodstuffs as an acid regulator and an aroma enhancer.

When the harmonisation legislation has been completed in the EU, the official number for fumaric acid will be E 297.

EXERCISE II

In 1928, Diels and Alder, two German chemists, reported a successful addition reaction of maleic acid anhydride with butadiene, C_4H_6 . The double $C=C$ bond of the unsaturated anhydride opens and forms a new bond with carbon atoms 1 and 4 of the butadiene. A new double bond forms between carbon atoms 2 and 3 of butadiene.

Assignment

II a. Write the reaction between maleic acid anhydride and butadiene in structural formulas.

II b. A similar reaction takes place with cyclopentadiene, C_5H_6 , instead of butadiene.

Give the reaction between maleic acid anhydride and cyclopentadiene.

In a review book about maleic acid anhydride, MA, published in 1982, there is the following passage on this type of reaction:

"This reaction is called the Diels-Alder reaction, diene synthesis, or the [4+2] cycloaddition reaction. The role that MA has played in this reaction along with other dienophiles cannot possibly be covered in a single chapter such as this. The impetus provided to synthetic organic research, particularly in the field of steroids,

polycyclic aromatics and alkaloids, by allowing a one-step ring closure, can barely be exemplified in a treatment such as this."

The Diels-Alder reaction is seen by the authors as very important. Other compounds with molecules in a conjugated system of carbon-carbon bonds seem to react with maleic acid anhydride or chemicals with a comparable structure more easily, i.e. faster, and at a 'normal' temperature.

The Diels-Alder reaction is especially important for synthesis in pharmaceutical and agro-chemical industries. The former is interested in the synthesis of eg. steroids for medical treatment, and the latter in the synthesis of eg. crop protection chemicals. Chemical research in these industries today uses molecular modelling, which is making calculations on computerised models of molecules. However, the foundations of this research were laid in a completely different way, by systematically investigating how chemicals react with each other and recording what happened.

In 1930, Theodor Wagner-Jauregg under the direction of Richard Kuhn examined Diels-Alder reactions of maleic acid anhydride with a series of diphenylpolyenes, dissolved in xylene. The first of the series, 1,2-diphenylethene (stilbene, $C_6H_5-CH=CH-C_6H_5$) did not react as expected.

Assignment

II c. Is it possible to obtain a Diels-Alder reaction by heating stilbene and maleic acid anhydride?

There was however a reaction product: a chemical described as "amorphous and high molecular" and "possibly built in chain form". They concluded that they had produced a polymer from an addition reaction between two monomers, maleic acid anhydride and stilbene.

Assignment

II d. Draw the structural formula of a part of the addition polymer formed from maleic acid anhydride and stilbene.

II e. See if you can think of any other possible structural formulas for II d.

In an article published later that year, Wagner-Jauregg suggested calling this a hetero addition polymer (these days it is called a copolymerisation product). He reports that the carbon and hydrogen content of the reaction product have been measured³. It contains 77.38 mass percent of carbon and 5.13 mass percent of hydrogen. Wagner-Jauregg concluded that the reaction product was a copolymer incorporating an equal amount of maleic acid anhydride and stilbene.

Assignment

II f. Calculate whether this conclusion coincides with the measured mass percentage.

When Wagner-Jauregg added maleic acid anhydride and stilbene in a mol ratio of 1 : 2, a reaction product resulted with almost the same carbon-hydrogen content as with the reaction with the mol ratio of 1 : 1 or 2 : 1. He concluded therefore that in a polymer chain maleic acid and stilbene do not occur in a random order but are organised neatly in an alternating formation.

Assignment

II g. Explain whether you agree with this conclusion.

Today, polymerisation with maleic acid anhydride, MA, and styrene (phenylethene) has been performed on a large scale; the polymer formed is known as SMA.

³ This was done in 1930 in more or less the same way as Pelouze did it in 1834.

Assignment

II h. Draw a part of a SMA molecule built from styrene and maleic acid anhydride monomers.

II i. Which properties do you predict for this polymer. Pay attention to the form of the molecules and to the other reaction possibilities.

Half of the yearly production of maleic acid anhydride is used to make other types of polymers. When the anhydride is heated with glycol (1,2-ethanediol), a copolymer is formed that appeared to have the same structure as the reaction product of glycol and maleic acid.

Assignment

II j. Draw the structural formula of a part of the polymer formed from maleic acid and glycol.

II k. This polymer can react further with styrene.

Draw a structural formula of a part of the product thus formed.

II l. What properties would you expect this product to have, as compared with SMA, the product mentioned in question II h ?

II m. What relationship do you see between the structures of these polymers and the possibility of recycling the two products?

In question II j you have used maleic acid as the monomer, but in reaction processes using anhydrides has some advantages: no water is released during the reaction, the reaction develops more quickly, and it is cheaper. One application for saturated polyesters like those formed by hardening with styrene is as a construction material, often in conjunction with fibre glass, in boat building for example.

7. NOW YOU HAVE MADE THE ACQUAINTANCE OF A COMPOUND

This brings us up to contemporary chemistry, from Pelouze's chemistry via the structures of Van 't Hoff, the Lewis theories and the crystallographic methods used by Yardley. You got better acquainted with two chemical compounds, and you have also experienced how this knowledge was built up and that it is still growing. The story of the two acids is not finished yet. New questions are thrown up all the time: theoretical questions, practical questions, questions about structures, questions about aspects concerning energy and applications and safety. People who want to answer these questions and many others work in all sorts of functions in different places all over the world. The diversity of the professions involved is demonstrated by the following list of people living in the Netherlands and Belgium who have contributed to the story:

Pharmacist in Wouw

Librarian of the Institute of Toxicology and Food in Zeist

General Manager Specialty Compounds in Genk

Teacher Hotel and Catering Institute in Middelburg

Research Manager Industrial Resins in Zwolle

Senior Policy Maker Ministry of Health

Senior Research Fellow Industrial Resins in Zwolle

Senior Lecturer in Crystal and Structural Chemistry in Utrecht

Section Leader Microbiology/ Biochemistry in Geleen

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Samenvatting

Dit proefschrift bevat een verslag van chemiedidactisch onderzoek betreffende het onderwerp Chemische binding in de zesde klas van het voorbereidend wetenschappelijk onderwijs (6vwo). Het onderzoek werd uitgevoerd bij de Vakgroep Chemiedidactiek van de Universiteit Utrecht gedurende de periode 1990-1995. Mijn belangstelling voor het onderwerp kwam voort uit vragen ten aanzien van het onderwijzen van atoombouw als inleiding tot het onderwijzen van chemische binding. Deze vragen speelden al tijdens mijn werk als chemiedocent en als lid van de Gebruikersredactie van CHEMIE (Wolters-Noordhoff). Ze zijn opnieuw relevant geworden in verband met de komende veranderingen in de bovenbouw van het voortgezet onderwijs.

Chemische binding is in 6vwo traditioneel een onderwerp waarin chemische begrippen, theorieën en modellen aangeboden worden als voorbereiding voor de universitaire chemiestudie. De chemische inhoud is misschien minder relevant voor diegenen die geen scheikunde gaan studeren. De vaardigheid om met modellen om te gaan is daarentegen nuttig voor een ieder die zich universitair wil bekwamen. In de praktijk blijken leerlingen en docenten bij het leren en onderwijzen van chemische binding moeilijkheden te ondervinden. Onderzoek dat zich op het leren en onderwijzen van chemische begrippen en werkwijzen richt, chemiedidactisch onderzoek, is geschikt om uit te maken of deze moeilijkheden verband houden met een (gemis aan een) bepaalde begrippenstructuur, of anderszins samenhangen met de aangeboden inhoud. Daarbij kan didactisch onderzoek bijdragen naar het zoeken van oplossingen voor de moeilijkheden.

Chemiedidactisch onderzoek vindt plaats op het gebied van chemie en dat van chemie-onderwijs en richt zich met name op de wisselwerking tussen deze beide gebieden. Het hier gerapporteerde onderzoek kende twee doelen: ten eerste het uitvoeren van een didactische analyse van chemische binding en ten tweede het ontwikkelen van een didactische structuur van chemische binding.

Bij een *didactische analyse* worden betekenissen van chemische begrippen en werkwijzen bestudeerd in onderlinge samenhang en in hun relevantie voor het onderwijzen en leren van chemie. Het onderzoeksgebied van de didactische analyse is de chemische praktijk van chemici in wetenschap en industrie, en die van docenten, studenten, geschiedkundigen, wetenschapsfilosofen, schoolboekauteurs en anderen op dit terrein.

Een *didactische structuur* komt tot stand door het verwerken van de resultaten van de didactische analyse tot en het vervolgens uitvoeren van didactische experimenten. Chemische begrippen en hun onderlinge relaties worden in de didactische structuur ten behoeve van onderwijs beschreven aan de hand van resultaten uit de didactische experimenten wat betreft de onderwijsbaarheid en de leerbaarheid van deze begrippen.

Voor het uitvoeren van een didactisch experiment is het gebruikelijk een experimentele lessenserie te ontwerpen. In het kader van het onderzoek Chemische binding in 6vwo was dit een experimentele lestekst getiteld 'Kenniss Maken, de biografie van een stof'. Hierin wordt een toepassing uitgewerkt van de moleculaire structuurtheorie binnen een wetenschappelijke context van mensen die kennis maken.

De lestekst is ontworpen als mogelijke alternatief voor de gebruikelijke benadering van chemische binding via de atoombouw. De keuze voor een andere introductie hangt samen met de voorgeschiedenis van het onderzoek. Voor het herzien van de schoolboekenserie Chemie ten behoeve van de derde druk, was besloten tot een gemeenschappelijk project van de Vakgroep Chemiedidactiek en de Gebruikersredactie van CHEMIE.

Dit project hield in dat het hoofdstuk "Atomen alleen en tezamen", Hoofdstuk 10 in de tweede druk van CHEMIE, geanalyseerd zou worden om te komen tot voorstellen ter bevordering van de samenhang van de chemische begrippen en voor een beter onderwijs van de geboden modellen. De resultaten van het project bestonden uit: een voorstel tot herziening van de tekst dat door de Gebruikersredactie vrijwel geheel overgenomen is in de derde druk van CHEMIE; en een onderzoeksvoorstel om nader in te gaan op het onderwerp chemische binding, met speciale aandacht voor het gebruik van modellen hierbij.

In de nu volgende hoofdstuksgewijze bespreking van de inhoud van het proefschrift geef ik een verantwoording van het onderzoek met inbegrip van de in dit kader ontworpen lessenserie 'Kenniss maken'.

Hoofdstuk 1 bevat de rapportage van de analyse van een aantal paragrafen over atoombouw en chemische binding uit de tweede druk van bovengenoemd schoolboek. De analyseresultaten laten ondermeer zien dat de beschrijving van de bouw van een vrij waterstofatoom niet voorbereid op de beschrijving van het tot stand komen van een binding in een twee-atomig waterstofmolekuul. Deze bron van verwarring is *breuk* genoemd. De breuk wordt op verschillende manieren beschreven, onder andere als een breuk tussen het model van een vrij atoom en dat van een gebonden atoom, en als een breuk ten gevolge van een fysische introductie met energieniveaus als voorbereiding op een beschrijving van chemische binding waarin posities van atomen relevant zijn. In het voorstel tot herziening van Hoofdstuk 10 is de volgorde gebleven, maar er is een verbeterde introductie van een eenvoudig afstand-energie model voor het vrije atoom opgenomen. Door voor het gebonden atoom een ander model aan te bieden is er de gelegenheid om verschillende modellen met elkaar te vergelijken.

De voor het didactisch onderzoek geformuleerde vragen laten twee motieven voor verder onderzoek zien: op welke wijze kan een chemische binding op een *chemische wijze* benaderd worden; en hoe kunnen leerlingen meer begrijpen van modellen en het omgaan met modellen aan de hand van een onderwerp als chemische binding.

In Hoofdstuk 2 wordt de didactische analyse voortgezet door na te gaan of de structuur van de elektronenwolk van een atoom ontwikkeld met ionisatie-energieën en energieniveaus het tot stand komen van een chemische binding tussen atomen aanneemelijk maakt. Argumenten worden aangevoerd dat dit niet het geval is en dat de beschrijving van de elektronenwolk gebaseerd op fysische gegevens niet consistent is met begrippen, als bijvoorbeeld valentie-elektronen, die voor een gebonden atoom nodig zijn. Dit leidt tot de constatering dat er sprake is van twee verschillende contexten en dat de breuk beschreven kan worden als die tussen een chemische en een fysische context.

De volgorde, eerst vrij atoom en dan gebonden atoom, komt niet alleen in andere schoolboeken voor maar eveneens in een veelgebruikt universitair studieboek. Deze introductie wordt in verband gebracht met de voorkeur voor een 'theorie eerst' benadering en met de reductionistische opvatting dat fysica, in het bijzonder de quantumtheorie, de fundamentele wetenschap is.

Ik voer aan dat niet alle chemici overtuigd zijn van de toepasbaarheid van de reductionistische benadering en dat vooral het begrip *chemische structuur* (of vorm) niet afgeleid kan worden uit quantummechanische 'first principles'.

■ laat zien dat in het Periodiek Systeem verschijnselen en theorieën uit zowel de chemische als de fysische context productief gecombineerd worden. Daarentegen blijkt dat de beschrijving van het vormen van een methaanmolekuul voornamelijk een combinatie is van verschijnselen en theorieën binnen de chemische context.

In dit hoofdstuk maak ik een onderscheid van twee stappen in een 'thesis of reduction', de eerste betreft de reductie van een verschijnsel tot een theorie en de tweede een reductie van de ene theorie tot een andere. Vervolgens voer ik argumenten aan voor meer aandacht in het onderwijsaanbod voor (chemische) verschijnselen ook als theorieën besproken worden. Uit argumenten voor een pluralistische opvatting van meerdere theorieën naast elkaar kom ik tot de keuze van een chemische benadering voor chemische binding.

In hoofdstuk 3 interpreteer ik de twee stappen van de 'thesis of reduction' met het accepteren van modellen en het gebruiken van modellen.

Bij het werken met molekulen en atomen moet eerst de hypothese geaccepteerd worden van de corpusculaire aard van materie. Pas daarna kunnen modellen van de corpuscula, molekulen en atomen, geïntroduceerd en gebruikt worden. Met het niet accepteren in de eerste stap verbind ik het onderwijsprobleem van molekulen als kleinste deeltjes van de stof. Drie methoden voor het introduceren van het gebruik van corpusculaire modellen worden beschreven in dit hoofdstuk: er wordt één model gepresenteerd, er is een opeenvolging van modellen waarbij het vorige model steeds verworpen wordt, en er is een benadering waarbij verschillende modellen naast elkaar gebruikt worden. Met deze laatste benadering komt *de betrekkelijkheid van een model* tot uiting.

Na het analyseren van het modelgebruik in een aantal schoolboeken geef ik een verdere beschrijving van het vrije atoom en het gebonden atoom. Het vrije atoom heeft als belangrijk modelkarakteristiek dat het vooral een energiecontext betreft, terwijl het gebonden atoom meer past in een afstandscontext.

Een vraag bij het ontwerpen van lesmateriaal is hoe door wetenschappers aanvaarde modellen door leerlingen in het onderwijs toch als betrekkelijk ervaren kunnen worden.

Hoofdstuk 4 bevat de overgang van de didactische analyse naar het didactische experiment in de cyclische onderzoeksprocedure van didactische analyse en ontwerpen, testen en evalueren van lesmateriaal.

Na de meer algemene beschrijvingen in de didactische analyse bespreek ik de keuzen die gemaakt zijn ten behoeve van het didactische experiment. Een van de keuzen is het introduceren van een chemische theorie, namelijk de *moleculaire structuurtheorie*. Vervolgens is gekozen voor het laten *ontwikkelen van een structuurformule* als middel om de betrekkelijkheid van een model te onderwijzen. Een structuurformule is zowel een weergave van de eigenschappen van de desbetreffende stof als een model van een molecuul van die stof. Afhankelijk van het gebruik van de structuurformule moet men zich steeds realiseren welke betekenis streepjes en elementsymbolen in zo'n formule kunnen hebben.

Zo zijn voor het didactische experiment keuzen gemaakt om bepaalde chemische begrippen in het onderwijs aan te bieden. Daarbij worden deze begrippen uit hun oorspronkelijke context gehaald. Dit heb ik decontextualiseren genoemd. Voor het nieuw te ontwerpen onderwijs moet er een nieuwe, adequate, context aangebracht worden waar deze begrippen zoveel mogelijk hun betekenis houden. Dit noem ik recontextualiseren.

Voor het ontwerpen van het lesmateriaal heb ik richtlijnen gezocht in beschouwingen over wetenschap, in regels voor het schrijven van wetenschappelijke teksten en in principes met betrekking tot het schrijven van een historisch verhaal. De gevonden drie richtlijnen zijn respectievelijk een *leidend principe*, een *samenhangende volgorde* en een *overkoepelende context*. Daarnaast is gekozen voor het onderwijzen van in de wetenschap aanvaarde kennis op een manier die de werkwijze van wetenschappers nabootst als deze nieuwe kennis maken.

Hoofdstuk 5 bevat het verslag van het ontwerpen van de experimentele lestekst en van het eerste experiment met deze lestekst in enkele klassen.

De drie genoemde richtlijnen gebruik ik om het ontwerp van de lestekst te beschrijven. Het leidend principe is de keuze voor het 'vanuit-de-stof denken'. Dit betekent dat zoveel mogelijk ook bij de theoretische beschouwingen experimentele chemische en fysische gegevens een rol spelen. De moleculaire structuurtheorie is als samenhangende volgorde op te vatten en de overkoepelende context is die van mensen die 'kennis maken'.

De lestekst heeft als inhoud het ontwikkelen van structuurformules, ondersteund door een verhaal in episodes. De episodes zijn tezamen met opdrachten bedoeld om het proces van wetenschappelijk kennis maken te laten ervaren. Er is gekozen voor een stoffenpaar zodat het steeds noodzakelijk is een nieuwe representatie op te stellen om de individuele stoffeigenschappen te kunnen beschrijven.

De aanvankelijk intuïtieve keuze van de twee verwante stoffen, maleïnezuur en fumaarzuur, als voorbeeld om een aantal chemische begrippen te behandelen heeft de volgende voordelen:

- leerlingen in 6vwo kunnen de nieuwe kennis over het stoffenpaar interpreteren en in verband brengen met hun bestaande kennis;
- de keuze voor twee verwante stoffen geeft mogelijkheden voor vergelijkingen en voor het moeten weergeven van verschillen (anhydridevorming) en overeenkomsten (chemische samenstelling);
- er zijn verschillende experimenten mogelijk geschikt voor een schoolpracticum;
- beide stoffen zijn relevant in hedendaagse industrie, ondermeer die van kunststoffen en voedingsmiddelen;
- er is een overvloed aan publicaties zowel historisch als eigentijds waarmee het maken van kennis en het gebruik van modellen geïllustreerd kunnen worden;
- maleïnezuur en fumaarzuur zijn geassocieerd met verschillende belangrijke punten uit de moleculaire structuurtheorie. Bijvoorbeeld: de volgorde van verhoudingsformule-molekuulformule-structuurformule; verschillende functionele groepen, gewone en cis/trans isomerie; wederzijdse beïnvloeding van functionele groepen, intra- en intermoleculaire waterstofbruggen; verschillende soorten polymerisatiereacties; en structuureigenschapsrelaties.

De opdrachten in de lestekst geven de leerlingen de gelegenheid te discussiëren terwijl zij kennis maken zowel in de betekenis van het leren kennen van twee stoffen en hun reacties als het ervaren hoe de kennis omtrent de representaties tot stand is gekomen. Als onderzoeksmateriaal zijn gebruikt protocollen van deze discussies, verder schriftelijke uitingen van de leerlingen en mijn observatiesnotities gemaakt tijdens het experiment in de klassen. In de rapportage van het didactische experiment is de aandacht vooral gericht op de uitkomsten van dit experiment met betrekking tot een titratieopdracht. Deze opdracht houdt in dat via een zuur-base titratie een waarde gevonden moet worden voor n in de verhoudingsformule $(\text{CHO})_n$. Mede door het op verschillende manieren uitwerken van de titratie-opdracht is het mogelijk gebleken een interpretatie van chemische formules voor te stellen in termen van een massacontext, een afstandscontext en een ladingscontext.

Een voorlopige didactische structuur van moleculaire chemische binding is opgesteld door opeenvolgende stappen aan te geven in de ontwikkeling van een structuurformule in relatie tot de betekenis van streepjes, namelijk in een massacontext, in een massa+afstandscontext en in een massa+afstand+ladingscontext.

Hoofdstuk 6 geeft de overwegingen voor het herzien van de lestekst voor een tweede ronde van uitproberen in de klas. (Het resultaat van deze herziening is opgenomen als bijlage in het proefschrift.) Vervolgens komen twee onderwerpen uitgebreid aan de orde, namelijk de herziening van de slotparagraaf van de lestekst en het didactische experiment met een opgave over waterstofbruggen.

In het verslag van de herziening van de slotparagraaf geef ik aan hoe de verschillende richtlijnen een rol spelen tijdens het zoeken en selecteren van voor de lestekst relevant materiaal, en vervolgens voor het recontextualiseren van de gekozen begrippen. Een overkoepelende context van bijvoorbeeld maatschappelijke chemie zal andere eisen stellen dan een overkoepelende context van chemie als wetenschap.

De opdracht over waterstofbruggen heeft als resultaat opgeleverd dat in tekeningen van leerlingen verschillende betekenissen van streepjes in een structuurformule achtereenvolgens geïnterpreteerd kunnen worden als overgangen in betekenis van bij-elkaar-horen, van een ruimtelijke notie en van een bepaalde aantrekking. Hiermee hebben deze leerlingen een overgang gemaakt van betekenissen uit een massacontext, naar die in een afstandscontext en vervolgens in een ladingscontext. Het kunnen overgaan van de ene naar de andere context is geïnterpreteerd als het kunnen gebruiken van verschillende modellen naast elkaar.

In de afsluitende paragraaf van het hoofdstuk bespreek ik verschillende mogelijkheden voor verder chemiedidactisch onderzoek en voor verdere onderwijsontwikkeling.

Omdat de lestekst bestemd was voor leerlingen in 6vwo waarbij gebruik gemaakt kon worden van hun eerder verworven kennis op het gebied van organische chemie is een vervolgvraag hoe een lestekst er uit moet zien waarin deze kennis voor het eerst aangeboden wordt. Dus hoe de introductie van de moleculaire structuurtheorie kan plaats vinden.

Een andere vraag is of er meerdere volgordes van contexten in een didactische structuur mogelijk zijn en hoe de andere bindingstypen, hetzij afzonderlijk, hetzij in samenhang met de moleculaire structuurtheorie, geïntroduceerd kunnen worden.

Verder ga ik in op de mogelijkheden om lesteksten ontworpen voor didactisch onderzoek geschikt te maken voor implementatie op grotere schaal, dit mede in verband met de komende ontwikkelingen in het voorgezet onderwijs.

Dankwoord

*Teaching is asking questions with the answers known.
Researching is not knowing which questions to ask.*

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It kealtje leit yn 'e groppe.

Curriculum Vitae

Geeske M. van Hoeve-Brouwer werd geboren op 2 maart 1943 in Rotterdam. Na de lagere school in Bandung, Indonesia, doorlopen te hebben behaalde zij in 1961 het diploma gymnasium- β aan het Grotius Gymnasium te Delft. In hetzelfde jaar begon ze de studie scheikunde aan de Rijks Universiteit te Leiden, alwaar zij het kandidaats examen G in 1964 aflegde. Het doctoraal examen werd cum laude behaald in 1967 met als hoofdvak biochemie (Prof. L. Bosch), bijvak organische chemie (Prof. E. Havinga) en derde richting, fysisch-chemische scheidingsmethoden (Prof. C. J. F. Böttcher).

Naast het verrichten van werkzaamheden voor de Noord-Hollandse Uitgevers Maatschappij verkreeg ze in 1969 de lesbevoegdheid scheikunde. Van 1971 tot augustus 1990 was ze als (part-time) docent verbonden aan scholen voor voortgezet en hoger beroepsonderwijs in respectievelijk Zutphen, Oudenbosch, Etten-Leur en Bergen op Zoom, met als laatste school de RSG " 't Rijks" in Bergen op Zoom.

Van 1977 tot 1988 maakte ze deel uit van de Gebruikersredactie van de scheikunde serie CHEMIE voor vwo en havo (Wolters-Noordhoff). Ze was daarbij betrokken bij het voorbereiden van de eerste druk en het herzien ten behoeve van de tweede druk van de serie. Vanaf 1988 werkte ze mee aan een project ter voorbereiding van de derde druk van CHEMIE. Dit project betrof een samenwerking van de Gebruikersredactie en de vakgroep Chemiedidactiek van de Universiteit Utrecht.

Ze verrichtte vanaf augustus 1990 tot augustus 1995 in dienst van de Universiteit bij de Vakgroep Chemiedidactiek het onderzoek waarvan in dit proefschrift verslag is gedaan.

Als vertegenwoordiger van de NVON en de KNCV was ze lid van de Commissie Veldadvisering Leerplanontwikkeling (VALO) van 1988 tot 1992.

Van 1991 tot 1995 was ze bestuurslid van de Koninklijke Nederlandse Chemische Vereniging met als aandachtsgebied arbeidsmarkt en maatschappelijke taak.