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AUTHOR	Goedhart, Martin; van Duin, Yvonne
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ABSTRACT

Structural formulas give professional chemists information about physical and chemical properties of corresponding compounds. In chemistry education at secondary schools, structural formulas are introduced in the context of chemical bonding. Structural formulas are not introduced as representations of the properties of chemical compounds. This paper reports about a research project investigating how upper level secondary school students use the information that is given by structural formulas, especially with respect to the solubility of compounds in water. The investigations were based on a small-scale case-study approach, and information was obtained by recording discussions between students working in small groups. In the first round of the project, it was concluded that a great deal of students used rules of thumb (like "polar compounds dissolve in polar solutes"), but their argumentations were not complete and they seemed to lack understanding. A second round of research tried to provide students with an experiential basis concerning solubilities of organic compounds and let them formulate rules by themselves. Students formulated the rules intended readily. One of the problems met in this study is that some students did not show a proper understanding of the "functional group" concept. Based on findings, some recommendations are given for the teaching of structural formulas at the secondary school level. (Contains 22 references.) (Author/MM)

TEACHING STRUCTURAL FORMULAS IN CHEMISTRY

How students relate structural formulas

to the solubility of substances

Paper presented at NARST conference

March 29, 1999

Boston

Martin Goedhart & Yvonne van Duin

Research group of Chemical Education

University of Amsterdam

Nieuwe Achtergracht 129

NL - 1018 WS Amsterdam

The Netherlands

goedhart@chem.uva.nl

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Martin Goedhart & Yvonne van Duin

Research group of Chemical Education

Nieuwe Achtergracht 129

NL - 1018 WS Amsterdam

The Netherlands

goedhart @chem.uva.nl

Abstract

Structural formulas give professional chemists information about physical and chemical properties of the corresponding compounds. In chemistry education at secondary schools structural formulas are introduced in the context of chemical bonding. Structural formulas are not introduced as representations of the properties of chemical compounds.

In this paper we report about a research project in which it is investigated how upper level secondary school students use the information that is given by structural formulas, especially with respect to the solubility of compounds in water. Our investigations were based on a small-scale case-study approach. Our information was obtained by recording discussions between students working in small groups.

In the first round of the project it was concluded that for a great deal students used rules of thumb (like "polar compounds dissolve in polar solutes") but their argumentations were not complete and they seemed to lack understanding.

In a second round we tried to provide students with an experiential basis concerning solubilities of organic compounds and let them formulate rules by themselves. Studetns formulated the rules intended readily. One of the problems met in this study is that some students did not show a proper understanding of the 'functional group' concept. Based on our findings we give some recommendations for the teaching of structural formulas at secondary school level.

1. Introduction

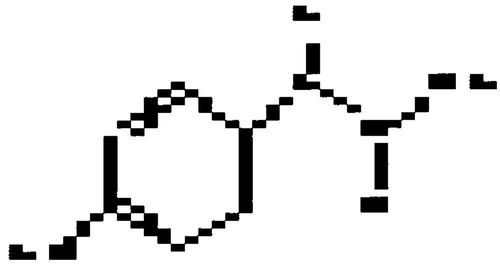
Structural formulas are among the most important tools of the professional chemist, especially in organic chemistry. As Weininger (1984) stated:

> *"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"*

We can see from this that a structural formula of a certain compound is to be considered as a reflection of known phenomena and on the other hand certain properties - not only chemical, as the text suggests, but also physical - can be predicted from it.

Structural formulas, in fact nothing more than letters coupled by lines, are representations of chemical compounds. These formulas not only give an impression of molecular geometry, but also give information about properties of the substances, such as chemical reaction possibilities and physical properties (a.o. melting and boiling point, solubility).

For instance, when we consider the structural fomula of a compound, like the well-known analgesic paracetamol:



then experts are able to give expectations about:

- its solubility in different solutes,
- its state of matter at room temperature and expected melting- and boiling points,
- its basic or acidic properties when dissolved in water,
- its reaction possibilities,
- its physiological significance,
- possible routes to synthesize paracetamol from other chemical compounds.

A structural formula is a condensed body of knowledge, just like other symbolic representations used in science, such as graphs and formulas that express the relations between quantities. Experts derive properties from structural formulas by considering different functional groups present in the structural formula (Woolley, 1988).

> *" 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 synthesize new substances. "*

So, in using structural formulas the functional group concept has a very central place. Functional groups bring order in the collection of letters and lines. In the paracetamol example a chemist distinguishes between the hydroxyl-, the amide-, the phenyl- and methyl-group and he uses his knowledge of group-properties relations to predict properties for this compound.

Despite the importance of structural formulas in chemistry not much research has been done on the teaching of this topic, probably because it is not known as a difficult subject for students. However, we had some indications that secondary school students interpreted the functional group concept in a different way than chemists do. This information came from our involvement with 'microchem', a large scale project aimed at the distribution of microscale glassware to Dutch secondary schools. At the moment about 300 schools (50 % of the total number of Dutch schools) participate in this project. In this project chemical experiments are developed and evaluated by our research group.

In this paper we focus on the relation of structural formulas and a certain substance property, namely the solubility in water. To be more precise, we investigated in what way students use the information supplied by structural formulas to make predictions about the solubility of certain compounds in water.

2. A perspective on teaching and learning

Research done in the field of science education during the last two decades has produced extensive knowledge about learners' conceptions with respect to natural phenomena and scientific concepts (Driver et al., 1985 ; Wandersee et al., 1994 ; Glynn and Duit, 1995). This inventarisation has led to the generally accepted view that there is a gap between the conceptions students have and intended learning outcomes.

Although promising suggestions have been made to bridge this gap, it seems that these attempts, when applied in the classroom, have not been very successful. In this paper we will present a perspective, which may contribute to a solution of this problem. First, we will mention two basic points of this perspective.

The first one is that we consider 'learning science' as a process of language development. The role of language is generally neglected by science educators: perspectives from cognitive psychology and philosophy of science seem to be dominant (see e.g. Duschl et al., 1990). Although the role of language is sometimes mentioned in so-called constructivist approaches, e.g. Driver mentions "negotiating of meanings" (Driver, 1988), language is considered as an instrument to exchange and clarify ideas, but conceptual development is not considered as a development of language. In our opinion, learning means language formation in a group of learners, putting into words their experiences, sharing their ideas, agreeing upon their meanings .... As we shall see this approach has important consequences for science education as well as for science education research.

The second point is that we start from the learner and not from educational objectives. We do not consider conceptions as wrong ideas that should be changed as soon as possible, but as a fruitful beginning of a learning process. We reject a curriculum, which has been constructed from the perspective of the scientist (or science teacher), resulting in a list of educational objectives about knowledge and skills to be mastered by the students. Premising the curriculum results in overburdenness of the school programme and in the inclination to "a forced conceptual development" (Lijnse, 1998), which results in learning problems and motivation problems of students, a situation well-known to science teachers. In this respect we agree with Driver that a curriculum should be viewed as "a programme of learning tasks, materials and resources which enable students to reconstruct their models of the world to be closer to those of school science" (Driver, 1988).

The challenge of our approach is to design sequences of teaching activities that are aimed to develop the language of learners. So, we choose a 'bottom-up' approach (Lijnse, 1998) in which the curriculum itself is the research object. The demands we make to such a curriculum are that the activities are permanently related to the abilities of the students and that it must lead to progress, i.e. that the students adopt, step-by-step, a scientific view on the world they experience.

The design and determination of a sequence of such teaching activities is not an easy task, but we use a model to organize teaching activitites in an explicit way. Our model is the Van Hiele level scheme (figure 1).

Ground level of phenomena

(argumentation with every day-words)

¬

Descriptive level of generalizations

(argumentation with words with an agreed meaning)

¬

Theoretical level of abstractions

(argumentation with words with a well-defined meaning)

Figure 1: Van Hiele level scheme

There are three levels: a ground level, a descriptive level and a theoretical level. We do not go into great detail about this scheme, which originates from the teaching of geometry (Van Hiele, 1986), but we mention here that the three levels correspond with different qualities of argumentation. At a ground level words do not have an agreed meaning. This situation is common in everyday life. We do not need a definition for 'table' to talk about tables and in most situations we do not meet communication problems.

The same applies to words used in science or mathematics, like 'square', 'substance' or 'force'. Most humans have an idea what is meant by these words. However, we may encounter situations in which we need agreement on the meaning of these words. Such a situation rises when someone asks whether a square is a rhombus. When such a question is asked in the classroom (This is really a strange question in everyday life. This must be a teacher's question!), students can mention properties of squares and discuss these (and of rhombuses, too). However, it is necessary to agree upon the meaning of the words used in these descriptions, like angle, side, diagonal, symmetrical and so on. This kind of agreements are characteristic for the descriptive level.

The list of properties of 'square' may grow and grow (right angles, equal sides, equal diagonals, diagonals intersect eachother perpendicularly etc.) and it seems that there is an indefinite number of properties without any order. For the students there may grow a need to bring order in this list and this is provided at the theoretical level. At the theoretical level we can give a definition of 'square'. A definition must be economical, unambiguous and comprehensive. We can see from this example that the meaning of square and rhombus have changed: at the ground level these are figures with certain visual shapes (but not described in words yet), at the descriptive level the figures are described by some properties (it is still represented by a certain shape), at the theoretical these are abstract objects defined by a number of properties.

An important point for teaching is that the levels have to be passed through subsequently. This means that experiences with phenomena have to precede generalized statements, and these have to precede abstractions. When the language of the theoretical level is introduced too soon students might learn this language but they lack understanding. For instance, beginning students in geometry do not understand why they need a definition for 'square' or beginning chemistry students do not understand why the particulate nature of matter is introduced. The consequence of this latter is that students properties are attributed to atoms and molecules which are not correct from a scientific view.

This example illustrates that the Van Hiele level scheme is useful both in the design of a curriculum and in the diagnosis of learning problems (Goedhart, 1999).

3. Research method

Our theoretical framework also has implications for research methodology, because when learning is considered as language development the consequence is that in our research work the language used both by students and teachers has to be analyzed. The purpose of this analysis is to monitor the progress in language development by learners and to work out which problems they meet with the assignments that are used in the teaching materials. In this way we are able to relate students' learning to the newly designed curriculum.

How do we start a research project within this research programme? Our starting point is the existing curriculum. In the classroom we record discussions between students and their teacher. These give information about the way students use the concepts learnt before and about the way new concepts are learnt. In many cases questionnaires and written tests are used as well. These findings lead to a reflection of the current teaching practice.

This, together with a thorough analysis of the concepts relevant in the field under investigation, is used to design a first version of a teaching sequence based on the Van Hiele level scheme. In this stage research questions can be stated more precisely. This teaching-development-research cycle is presented schematically in figure 2.

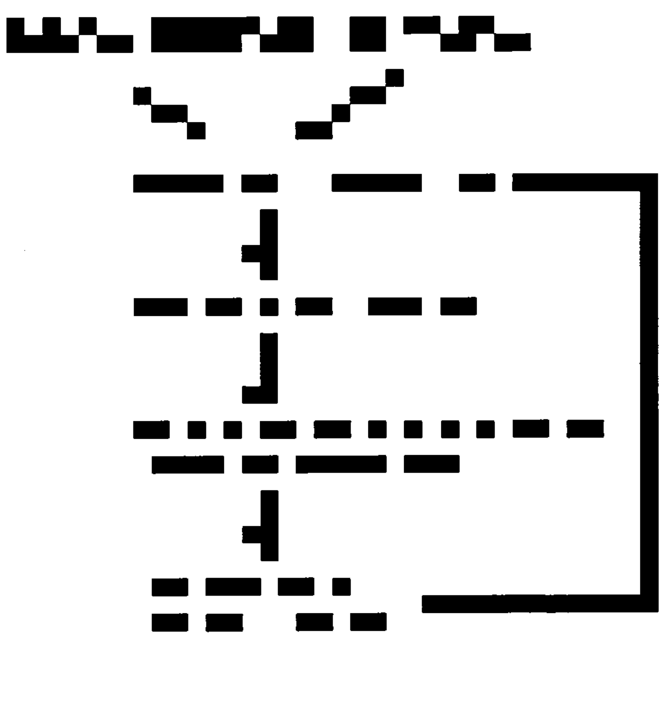


Figure 2: Teaching-development-research cycle

As we can see from this scheme our research methodology may be considered as a way to produce:

- data about teaching and learning,

- research questions,

- a new curriculum and teaching materials.

And moreover, the investigations are used to evaluate our theoretical framework, the Van Hiele level scheme.

In our approach teachers play an essential role. This means that at all stages of the research project they are involved (action research). Sometimes the researcher and the teacher are one and the same person. We think this is a profitable situation.

Our research approach is intensive and time-consuming. So, because of practical reasons the number of situations, which is incorporated in the study, is small. It has the nature of a case-study.

Our research approach should be evaluated by our aim "the development of a curriculum with which we detect the development of language in the direction of a scientific view". When we are able to show that such a curriculum is profitable, we are satisfied. However, because of the cyclic nature of the research project, research is considered as a never-ending process. The end is more or less arbitrary, and - in most cases - is determined by practical (and financial!) considerations.

This research programme has shown to be able to produce curricula for initial chemistry education (Ten Voorde, 1977) in secondary school, and at university level for thermodynamics (Kaper, 1997), chemical structures (Joling, 1993) and the statistical treatment of errors (Goedhart, 1991).

4. Introduction of structural formulas and the solubility of substances in schoolbooks

Both schools that were involved in the research project used the same chemistry book. It is the most frequently used textbook in chemistry for secondary schools in The Netherlands.

In this book structural formulas are introduced in the beginning of the second year that students have chemistry lessons. After the chemical bond has been introduced several types of bonding are distinguished: a.o. the covalent and the ionic bond. For molecular compounds, in which atoms are covalently bonded, students learn to draw Lewis structural formulas acoording to a set of rules based on the covalency of different atoms (carbon = 4 etc.).

In a next chapter inorganic ionic compounds (salts) are treated and rules are presented to predict the solubility of salts in water (e.g. sulphates dissolve in water, except barium-, lead- and calciumsulphate etc.).

In a later stage during this school year attention is paid to the interaction between molecules. At first only Van der Waals interactions are mentioned and these are used to explain physical properties of compounds, like the states of matter of substances and differences in melting or boiling points between comparable kinds of substances. The abnormal high boiling points of NH_3, H_2O and HF are explained by assuming stronger intermolecular interactions and this is used to introduce dipole molecules, the polar bond and the hydrogen bond as forms of intermolecular interaction, which are said to be stronger than the van der Waals forces.

After that, the miscibility of organic liquids with water is considered. To predict the miscibility from structural formulas the following rules are given:

> " Liquids of which the molecules can form hydrogen bonds mix well.
>
> Liquids in which only van der Waals bonds are present mix well"

The first rule actually means that liquids with an OH- or NH-group mix with water.

The role of the hydrocarbon portion of the molecule on the solubility in water is not discussed.

This approach to introduce structural formules and to treat the solubility of substances is not very different from other Dutch schoolbooks or American schoolbooks (Dorin et al., 1990 ; Smoot et al., 1990), although there might be differences concerning the order of treatment of the various concepts and the way rules are formulated. One difference is that in most textbooks rules like "polar substances dissolve in polar solutes, nonpolar substances dissolve in nonpolar solutes" (sometimes this rule is abbreviated to: "like dissolves like") is mentioned. This rule is not present in the Dutch chemistry book.

5. Research on the teaching of the solubility of substances

Most of the research work done in the field of the teaching of solubility of substances is related with students' conceptions of particles (Piaget & Inhelder, 1941 ; Prieto et al., 1989 ; De Vos, 1990 ; Slone & Bokhurst, 1992 ; Ebenezer & Erickson, 1996). In these studies young pupils were the object of study and the emphasis was on the dissolution process and the conservation of the chemical substance after dissolution.

Not much research has been done on the students' ability to predict solubilities of substances from general rules, especially not in the field of the solubility of organic compounds in water.

Also research concerning the relation between students' interpretations of structural formulas of organic compounds and the properties of these compounds seems to be not very popular. Even in the field of the introduction of structural formulas at secondary schools not much research work has been done. This is somewhat strange, because of the relevance of structural formulas in chemistry (see chapter 2).

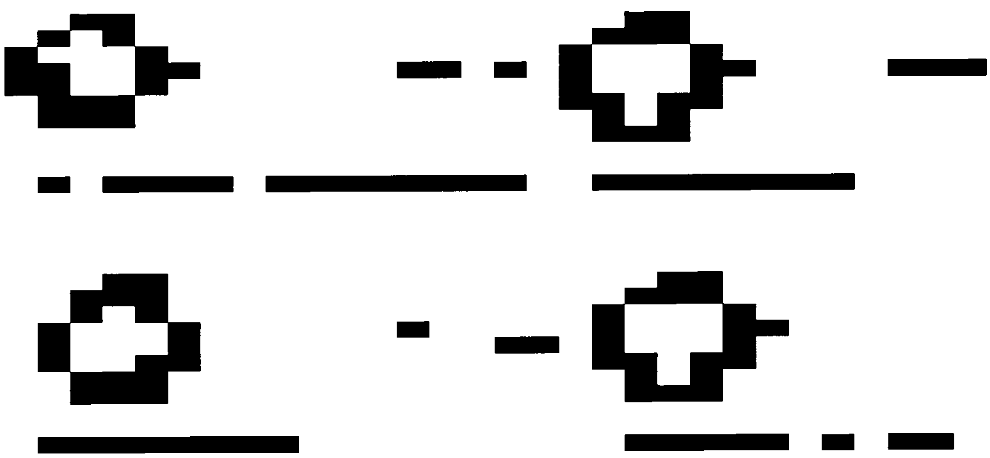
Van Hoeve-Brouwer (1996) has developed teaching materials in which 17-years old students draw conclusions about differences in structure between two isomers (fumaric acid and maleic acid) after they determined experimentally the differences in acidic properties of these two substances. However, this teaching took place some time after structural formulas were introduced, so that the outcomes should be considered as an assessment of students' understanding of the 'structure concept'.

In the next chapters we will present the findings of our research work done in this field. Two schools participated in this project. Resarch was done within the framework of our microscale project. Students worked in small groups (3-4 students) with a pilot experiment for our microscale manual (Goedhart et al., 1997).

6. The first round experiment

The first round of the research cycle was carried out at one school with 2 different teachers and 2 different groups of 4 students (pre-university level, 16 years old, 5th grade). These students were already acquainted with the rules given above. So our findings should be considered as an evaluation of the chemical knowledge they acquired before.

The experiment done by the students was the hydrolysis of methylbenzoate to benzoic acid. Questions were asked about the solubilities of compounds involved in this reaction.



First, students were asked for their expectations concerning the solubilities of methylbenzoate (the starting compound) and benzoic acid (the reaction product) in water (these are both insoluble). In one of the groups the discussion went as follows:

S2: Methylbenzoate, we have here, it reacts …

S1: … reacts with water, methylbenzoate reacts with it.

S3: It has to do with polar and nonpolar.

S1: Polar and nonpolar, yes, and what was …

S2: And polar, then it will dissolve, doesn't it?

S3: Water is polar. So, when it is polar it will dissolve.

S1: Then it is polar.

S2: Then it is polar.

S1: The first one is not, I think. Benzoic acid …

S2: I don't think so, too. So, it will, methylbenzoate will not dissolve, because it is …

S1: Benzoic acid is not … uh … it is polar too.

S2 Uuh?

T: Where do you look at when it is polar?

S1: No idea.

S2: Yes, minuses, I think.

We see that these students do not use structural characteristics to deduce the polarity of the compound and then give an expectation of its solubility in water, as was intended. Instead they seem to give an expectation without any clear argumentation, and then decide about the polarity of the compound. This means that the argumentation is reversed in comparison with the one intended.

We will see the same thing in the next two fragments:

S1: Are they soluble in water?

S2: Yes, I think they are soluble both. They are polar both.

S2: Polar, you know that, uh, benzoic acid, so that one will dissolve.

S1: That one dissolves well.

S2: We will write that down first.

Another conclusion drawn from the first fragment is that students applied the rule 'polar substances dissolve in polar solutes'. This is remarkable, because this rule is not mentioned in the textbook. The teachers manual even gives an advice against it. Apparently, the teacher has mentioned the rule in classroom before. This conclusion was supported by the fact that later in the discussion the teacher explicitly mentions the rule.

T: When does something dissolve well? Water is …

S1: Polar

T: … polar. Water is polar and these (substances) dissolve. So, which substances dissolve?

S2: When it is polar.

(……)

T: Polar mixes with … dissolves in polar and nonpolar in nonpolar.

When we look for the way students use the information given by structural formulas to deduce the polarity of molecules or the possible existence of H-bridges, then we can find hardly any argumentation that was given in the way it was given by the textbook. Some examples:

> S: That is ... with bonds, you know, when those bonds, uuh, are not equally strong. That has to do with it. Whether it is polar or not polar.
>
> S: This is a sodium salt and they all are soluble.
>
> S2: Alright, methylbenzoate is soluble.
>
> S1: Well, that depends, whether it can form H-bridges.

We found a lot of different argumentations. However, these had the nature of 'rules of thumb' and they hardly used characteristics of structural formulas in their argumentations.

Our challenge was to improve argumentations given by the students. We analyzed our findings with use of the Van Hiele level scheme. This framework gives us arguments why the traditional approach fails. General rules based on models seem to be introduced prematurely to these students. Students lack a solid basis at the ground level (experiences with solubilities of substances) and have not been involved in the formulation of these rules by themselves at a descriptive level.

This analysis also suggests the remedy for this teaching problem and that is an approach based on students' own experiences with solubilities and formulating their own rules. This approach has been tried in the second cycle of our research project.

7. The second round experiment

The second round of the research cycle was carried out at one school in two different classes (4th grade, 16 years old, senior general secondary education). In each class one group of two students was recorded on audiotape and observed; another group of two students was recorded on video.

In this experiment students were expected to develop their own rules on solubilities based on small experiments, in which organic liquids were mixed with water. All experiments were performed on microscale. It was intended that students recognize the role of the functional group and the length of the hydrocarbon chain on the miscibility of the (liquid) substances with water. By using graduated reaction tubes students were able to distinguish between totally miscible, partially miscible and immiscible with water. A summary of the experiments and the assignments given to students are presented in the appendix.

With respect to the role of the functional group students recognized the role of oxygen- and nitrogen atoms in combination with hydrogen atoms.

Some examples of rules students formulated:

- "the combination with H (OH, NH) makes compounds better miscible than other compounds."
- "when nitrogen or oxygen with a hydrogen bond is present solubility is high."
- "substances with OH-group or NH-group dissolve well."

With respect to the role of length and branching of the hydrocarbon chain formulation of the correct rule seldom gave problems. Some examples:

- "the longer the carbon chain the worse is the solubility".

- "The more branches a formula has, the better it dissolves"

Our approach was succesful because the formulation of rules did not gave problems in most cases.

However, in some instances we found that students experienced problems with the functional group concept. Despite the fact that the concept 'functional group' was already taught to these students, they did not seem to always have a proper understanding of this concept. Some examples from written protocols:

- "you have some O's there. So these O's have to do with solubility, don't you think? Because this one has only one and is less soluble that that one".

- (comparing the isomers methylpropanoate and 1-butanol): "This one has an O more and two H's less".

- (on a question about the solubility of glycol): " It is good miscible, because there is a H and this is not connected to a C".

- "What do you have to write down, the O is more left than in the other one?"

- "when the H is connected to the C it is not miscible."

Our conclusion is that these students did not recognize functional groups but identified separate element symbols instead. This for us unexpected result hampered the formulation of rules of solubility, in which the students were supposed to relate the presence of functional groups in structural formulas with the solubility of the corresponding substances in water.

We think that this phenomenon has been caused by the way the concept 'functional group' is introduced, namely as 'groups of separate atoms' and not as 'structural units reflecting substance properties'. So, for students the difference between esters and carbonacids is that some atoms are arranged in a different way, and not two classes of isomeric compounds with distinct chemical and physical properties.

8. Conclusions and implications for chemistry teaching

In secondary schoolbooks, a deductive approach is followed with respect to the introduction of structural formulas. This means that to students rules are presented to draw structural formulas, which are applied subsequently in exercises, like: "Write down the structural formulas of all isomers of C_5H_{12}. ". This is more a mathematical puzzle than a chemistry exercise. In our opinion this approach does not result in understanding structural formulas as representations of chemical properties. Problems may rise when students have to deduce properties of organic substances from structural formulas. This was illustrated by some of our findings in this research project. In many cases students did not deduce their expectations from structural characteristics, and when they did, their reasonings were incomplete. Frequently students used rules of thumb. We do not reject the use of rules of thumb, but in this case they cover up lack of understanding. Using the Van Hiele level scheme our interpretation is that generalisations, based on models, are introduced prematurely in chemistry lessons.

Our remedy is to offer students experiences with the solubility of substances, enabling them to formulate rules by themselves. Our second round experiment may be considered as an attempt to provide students with a phenomenological basis (Van Hiele's ground level) and involve them with the formulations of rules on solubility (Van Hiele's descriptive level). We hope to achieve that this results in a stronger relation between structural formulas and properties of compounds.

We argue in favour of a more phenomenological approach in chemistry education, in which students interpret phenomena and formulate generalizations themselves.

9. Literature

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APPENDIX: summary of solubility experiments

A. Comparison of different substances

Name of substance	Structural formula	Volume that mixes with water (mL)
butane	CH_3-CH_2-CH_2-CH_3	0
1-aminobutane	CH_3-CH_2-CH_2-CH_2-NH_2	0.5
butanoic acid	CH_3-CH_2-CH_2-C-OH O	0.5
1-butanol	CH_3-CH_2-CH_2-CH_2-OH	...
1-chlorobutane	CH_3-CH_2-CH_2-CH_2-Cl	...
1-bromobutane	CH_3-CH_2-CH_2-CH_2-Br	...

Questions:

•Which substances mix totally, partially or not with water?

• Which groups do these sunstances have?

• Order the groups according to decreasung solubulity.

B. Comparison of isomers with different functional groups

Name of substance	Structural formula	Volume that mixes with water (mL)
1-butanol	CH_3-CH_2-CH_2-CH_2-OH	...
ethoxyethane	CH_3-CH_2-O-CH_2-CH_3	...

Name of substance	Structural formula	Volume that mixes with water (mL)
	CH_3-CH_2-CH_2-C-OH	

butanoic acid	O	0.5
methylpropanoate	CH_3-CH_2-C-O- CH_3 O	...

Questions:

• What do you notice when you compare the functional groups of 1-butanol and ethoxyethane, and of butanoic acid and methylpropanoate?

• Formulate a rule concerning solubilities of these pairs of substances.

C. Comparison of alcohols with different carbon chain length

Name of substance	Structural formula	Volume that mixes with water (ml)
methanol	CH_3-OH	...
ethanol	CH_3-CH_2-OH	...
1-propanol	CH_3-CH_2-CH_2-OH	...
1-butanol	CH_3-CH_2-CH_2-CH_2-OH	...
1-pentanol	CH_3-CH_2-CH_2-CH_2- CH_2-OH	...
1-hexanol	CH_3-CH_2-CH_2-CH_2- CH_2- CH_2-OH	...

Question:

• Formulate a rule about solubilities of these substances.

D. Comparison of isomeric alcohols with differently placed OH-groups

Name of substance	Structural formula	Volume that mixes with water (ml)

1-butanol	CH_3-CH_2-CH_2-CH_2-OH	...
2-butanol	CH_3-CH_2-CH-OH CH_3	...
2-methyl-2-propanol	CH_3 CH_3-C-CH_3 OH	...

Questions:

- Formulate a rule about solubilities of these 3 substances.

- What do you expect to be the solubility of:

glycerol

glucose

2-methyl-1-propanol

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M. Goedhart and Y. van Duin

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Dr. Martin J. Goedhart (Associate Professor in Chemistry Education)

Organization/Address: Telephone: Fax:
AMSTEL instituut
Universiteit van Amsterdam
Kruislaan 404
NL-1098 SM Amsterdam
The Netherlands
tel. ++3120 5255886
fax ++3120 5255866

E-mail Address:
goedhart@science.uva.nl

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