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## **STRUCTURAL UNITS AND CHEMICAL FORMULAE**

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**ABSTRACT:** Teaching inorganic chemistry for beginners and introducing chemical formulae is not usually supported by structural models, while such models (e.g. the ball-and-stick model) are used in organic chemistry. On the basis of Dalton's atomic theory, we propose to take sphere packings and crystal lattices as structural models of inorganic solids. Students can develop images of chemical structures and differentiate between molecules and giant structures. Unit cells can be introduced as smallest units of giant structures, and students can derive formulae from given unit cells. Based on the above proposal, a research study was carried out with two classes of grade 8 as the experimental group and other three classes as control group. The experimental group was working for a period of about three months with metals, alloys and their chemical structures, finally with elementary cubes of the cubic structures and their unit cells. Performance in tests, coupled with answers to questionnaires and interviews showed that students of the experimental group were able to recognise unit cells of cubic structures and to derive empirical formulae from the used models. [*Chem. Educ. Res. Pract. Eur.*: 2002, 3, 185-200]

**KEY WORDS:** *structural chemistry; chemical structure; molecular structure; crystal structure; unit cell; chemical symbols; images; spatial ability; science literacy*

### **INTRODUCTION**

Understanding chemistry means knowing about properties of substances and how these relate to chemical structure and chemical bonding: these aspects are not separable. For beginners it is possible to catch the idea of structural models on the basis of Dalton's atomic theory. The concept of chemical bonding will be introduced later, after one or two years of chemistry instruction, on the basis of the nucleus-shell model of the atom, and will complete a sufficient understanding.

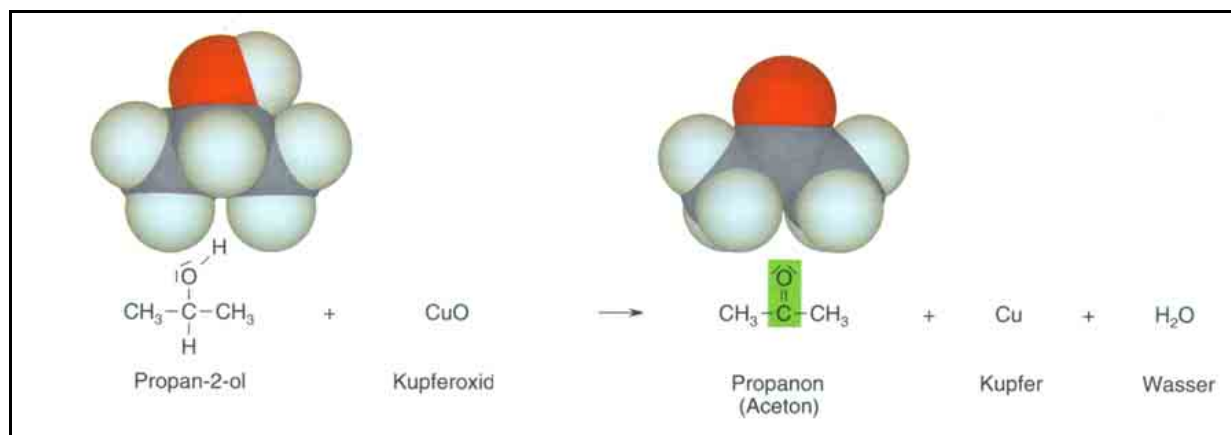
Teaching chemistry means discussing substances, their properties and reactions on the macroscopic level and structural models on the submicroscopic level. Taber (2001) speaks of the 'molar level' and 'molecular level'. Johnstone (2000) thinks of three corners of a 'chemical triangle', marking each corner with 'macro', 'submicro', and 'representational': symbols, formulae, equations, molarity, mathematical manipulations and graphs. He warns: "*It is psychological folly to introduce learners to ideas at all three levels simultaneously. Herein lies the origin of many misconceptions. The trained chemist can keep these three in balance, but not the learner*". Gabel (1999) states with regard to Johnstone's triangle: "*The primary barrier to understanding chemistry, however, is not the existence of the three levels of representing matter. It is that chemistry instruction occurs predominantly on the most abstract level, the symbolic level*".

**TABLE 1:** *Structural images - mediator between phenomena and chemical symbols.*

MACRO PHENOMENA	substances and their properties	chemical reactions
↓	↓	↓
SUBMICRO PHENOMENA		
structural images	structural models of substances, smallest units of structures	structural models of substances before and after reaction
↓	↓	↓
chemical symbols	symbols of smallest units of structures, chemical formulae	structural formulae in chemical equations, chemical equations

Therefore we teach “all three corners” one after the other (Barke, 1997): ‘macro level’ first, structural models on “submicro level” afterwards, finally chemical symbols (see Table 1). Chemical formulae should be considered as shortened models of the structure of substances on the submicro level, structural models could even be regarded as mediators between phenomena and chemical symbols - to avoid the predominance “on the most abstract level, the symbolic level”.

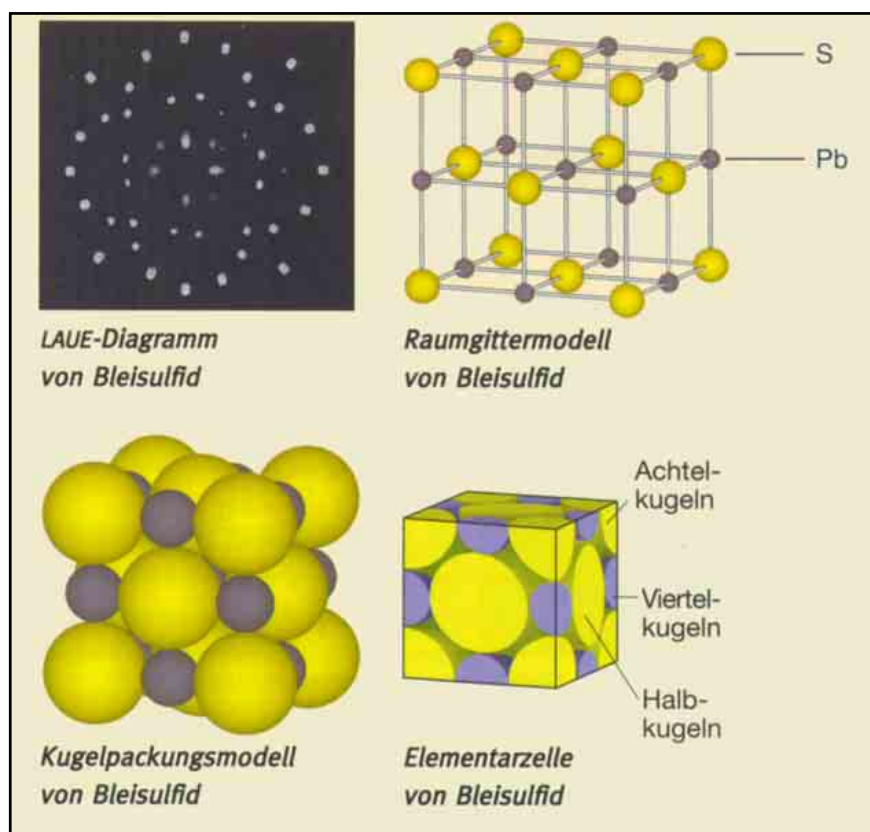
In organic chemistry it is useful to have ball-and-stick models or space-filling models of molecules and to derive structural formulae (see Figure 1). The models are also useful for discussing and understanding the different meanings of structural or molecular formulae. In every case these formulae represent the composition of the smallest units of volatile substances – in our example the composition of propanol and propanone molecules.



**FIGURE. 1:** *Description of the reaction of propanol to propanone on different levels: structural models, structural formulae, names (German language, Asselborn, Jäckel, & Risch, 2001, p. 313).*

## MOLECULES AND UNIT CELLS AS SMALLEST UNITS OF STRUCTURE

The idea of molecules as smallest particles or smallest units of gases is very obvious: students like this idea so much that they apply it to every substance, they even like to speak about ‘NaCl molecules’ in sodium chloride (Taber, 2001). But what are the smallest units of metals, salts and other high melting solids? What about the structure and the smallest units of ‘CuO’ and ‘Cu’? – Why don’t the authors show us structures of copper oxide and the metal coppers? (see Figure 1)



**FIGURE 2:** X-ray diagram, ball-and-stick model, elementary cube and unit cell of lead sulphide (sodium chloride structure) (Barke, 2001, p. 127)

**TABLE 2:** Counting the unit cell and deriving formulae of lead sulphide (see Figure 2).

<p><b>Pb atoms:</b></p> <p>12 atoms on edges: <math>12 \times 1/4 = 3</math> atoms</p> <p>1 atom in the centre: <math>1 \times 1/1 = 1</math> atom</p> <p>total: 4 atoms</p>	<p><b>S atoms:</b></p> <p>6 atoms on faces: <math>6 \times 1/2 = 3</math> atoms</p> <p>8 atoms on corners: <math>8 \times 1/8 = 1</math> atom</p> <p>total: 4 atoms</p>
<p>results: formula of the unit cell <b>Pb<sub>4</sub>S<sub>4</sub></b>,</p>	<p>Empirical formulae <b>Pb<sub>1</sub>S<sub>1</sub> or PbS</b></p>

On another page of their book (Asselborn, Jäckel, & Risch, 2001), the authors take lead sulphide as an example of salt structures and show the unit cell as the smallest unit (see Figure 2). They propose to count the parts of spheres within the unit cell to derive formulae. (see Table 2): Pb<sub>4</sub>S<sub>4</sub> as the formula of the unit cell, Pb<sub>1</sub>S<sub>1</sub> or PbS as shortened rational.

This approach has two big advantages. Firstly it helps students to understand where structures come from: the teacher can give the idea of X-ray analysis by using laser-beam experiments (Barke, 1990). Secondly students can develop mental images according to the structure of salts and other solids (see Table 1). They can grasp the difference between molecules and unit cells as smallest units and will avoid mistakes such as thinking of 'NaCl molecules' in sodium chloride or 'Li<sub>2</sub>O molecules' in lithium oxide (Taber, 2001). Thirdly they derive formulae from unit cells, i.e. by counting the unit cell of lead sulphide and arriving at Pb<sub>4</sub>S<sub>4</sub> or PbS (see Table 2 and Figure 2). If the concept of ions is available, sulphides, oxides or chlorides can be described with ions as their particles and with ions in unit cells.

The advantage seems to be the connection between mental images of chemical structures and relevant formulae. Traditional concepts usually take the historical way to derive formulae, by comparing masses of substances and atomic masses, or by comparing volumes of gases and using numbers of particles by Avogadro's law. Both ways to derive formulae are very demanding lessons and students of the age of 14-16 years are not happy with these mathematical manipulations. We will propose another way based on basic particles of matter and their combinations.

### ATOMS AND IONS AS BASIC PARTICLES OF MATTER

The Greek philosophers of the antiquity had a dream to discover the basic particles of matter and to combine them to give substances: "water, air, soil and fire" were the first aspects of their theory. Today we know that atoms and ions of the elements are these basic particles of matter! Therefore we propose to give students a list of atoms and ions on the basis of Dalton's atomic theory and the PSE, the periodic system of elements (see Figure 3). They also will be given rules to combine these particles mentally (see Table 3). The idea of ions may be introduced by experiments demonstrating decreasing melting points of salt solutions compared to solutions of molecular substances (Barke, 1992), and by experiments of electrical conductance or electrolysis.

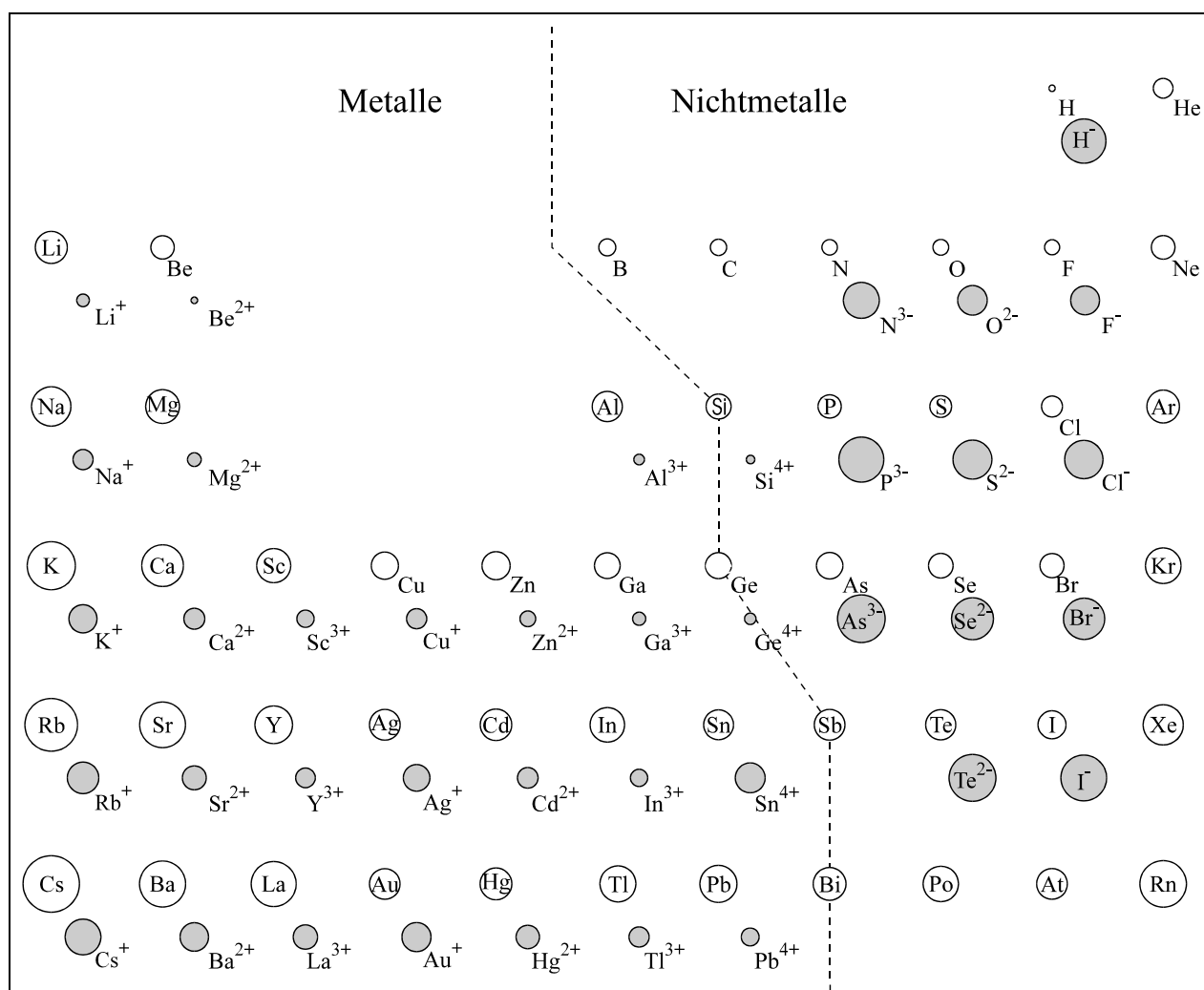


FIGURE 3: Atoms and ions as basic particles of matter (Sauer mann & Barke, 1997).

**TABLE 3:** Rules for combining atoms and ions according to the periodic table of the elements.

Place of particles in periodic table	quality of particles	combination
“left and left”	metal atoms	metal lattices
“right and right”	nonmetal atoms	molecules, atomic lattices
“left and right”	ions	ionic lattices

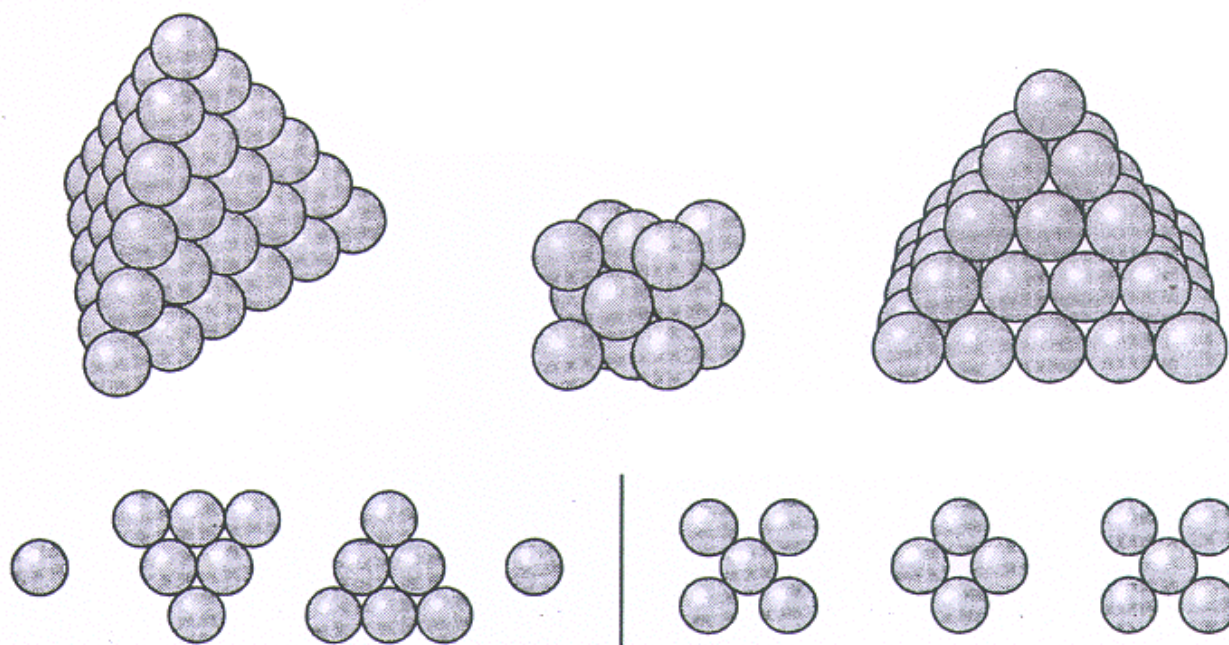
With the idea of listed atoms and ions as basic particles, students can combine them in their mind to form big structures (see Figure 3 and Table 2): metal atoms to metal lattices in metals and alloys (“left and left” in PSE), nonmetal atoms to molecules of volatile substances (“right and right” in PSE), and ions to ionic lattices in salts (“left and right” in PSE).

By using molecular building sets it can readily be shown how to combine C, H, and O atoms to form molecular structures of many organic substances. Because we place H atoms on the right side of PSE, all these well-known combinations can be indicated as “right and right in PSE”. Combinations of metal atoms “left and left in PSE” are not so usual - so let us describe the idea of combining metal atoms to metals and alloys in a more detailed way, especially with the aim to report our research findings on the basis of our curriculum.

### Metals

If we ask students to pack spheres closely together (close packing), they start (from our experience) to arrange them in a triangle or in a square pattern and will further pack layers on it as close as possible - like the salesman of fruits in the market packs his oranges. Children will get close packings like a tetrahedron or a pyramid (see Figure 4).

In both packings you can try to find the elementary cube built of 14 spheres: in the tetrahedron packing, by layers with  $1 + 6 + 6 + 1$  spheres; in the pyramid packing, by layers

**FIGURE 4:** Two forms of building the cubic closest packing of spheres and the elementary cube.

with  $5 + 4 + 5$  spheres (see Figure 4). You will also find the coordination number 12 in both packings: one sphere in the middle of the packing is touched by 12 other spheres in both packings. Both arrangements of spheres are identical: they have the same coordination number and the same cubic symmetry. Because the same containing elementary cube has one sphere on each face of the cube, this structure (as well as cubic close packing) is also called face-centred cubic structure.

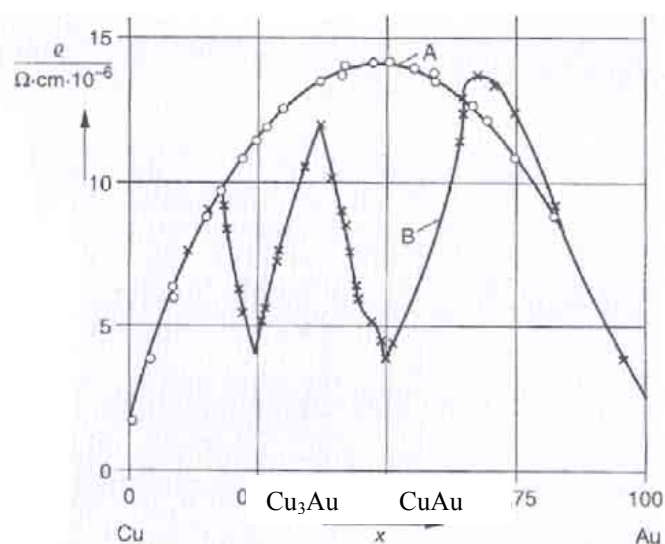
This structure is realised in nature by many metals: copper, gold and all precious metals, lead, aluminium, etc. There exist two other structures of metals: the hexagonal close packed structure (e.g. in magnesium and zinc), the body-centred cubic structure [e.g. in wolfram (tungsten) and the alkali metals].

To illustrate all three structures it is profitable to have about 50 spheres of the same size and to form packings and elementary cubes (see Figure 4). There are also building sets to build up sphere packings of many crystal structures. One of the best is the "Solid-State Model Kit" (Lisensky, Covert, & Mayer, 1994). The instruction manual describes further how to construct 'unit cells' of some important structures (compare in this regard elementary cube and unit cell in Figure 2): "Because the spheres supplied in the ICE Solid-State Model Kit cannot be divided into fractions, the kit cannot be used to construct a structure's unit cell without having parts of some spheres extend outside the actual unit cell. The directions 'to build a unit cell' will actually build the smallest collection of spheres and layers that *contain* a single unit cell" (Lisensky, Covert, & Mayer, 1994, p. 8).

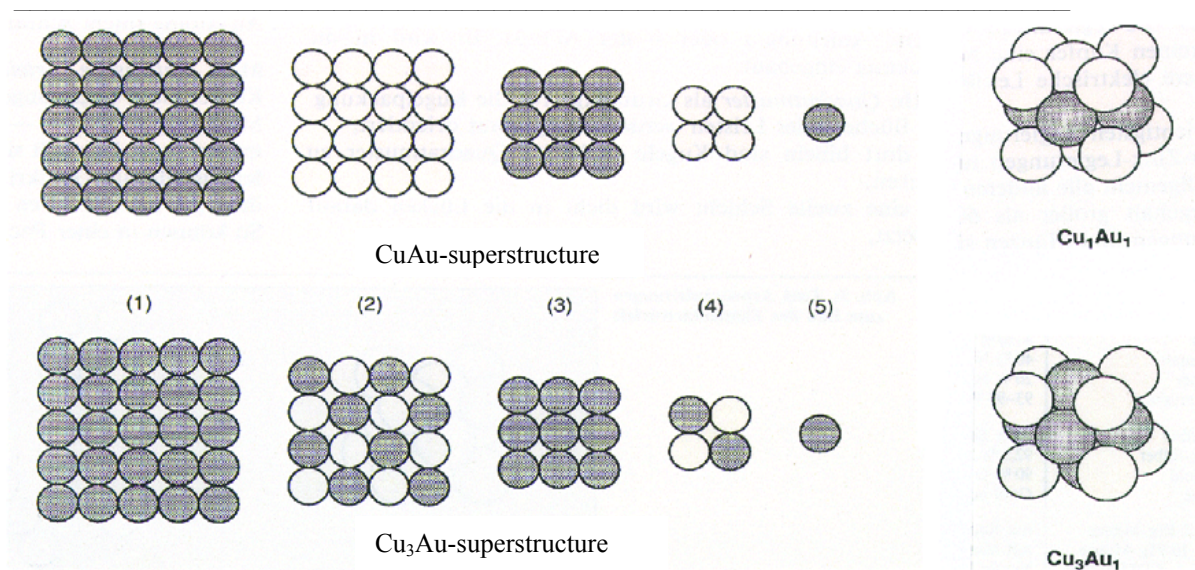
## Alloys

There is a very interesting example of an alloy: the copper-gold system. Both metals realise the same face-centred cubic structure and contain atoms of nearly the same size. So you can melt and mix both metals in every ratio: by cooling down you will also get crystals of every ratio from 0-100% copper or gold. The explanation is easy: Cu atoms and Au atoms of same size can be replaced at any place in their face-centred lattice, the substitution can take place randomly in every ratio. For illustration you can take spheres of the same size but of two colours and pack them randomly distributed in a face-centred cubic packing (see Figure 4).

Why is the Cu-Au-system so interesting? There are two special superstructures that can be described with  $\text{Cu}_3\text{Au}$  and  $\text{CuAu}$ . These special structures have a very high electric conductivity or a low specific resistance compared with all the other randomly ordered structures (see Figure 5): when all Cu-Au melts are cooled down very fast, you will get



**FIGURE 5.** Minima of specific electrical resistance of superstructures  $\text{Cu}_3\text{Au}$  and  $\text{CuAu}$  (Weiis, 1983).



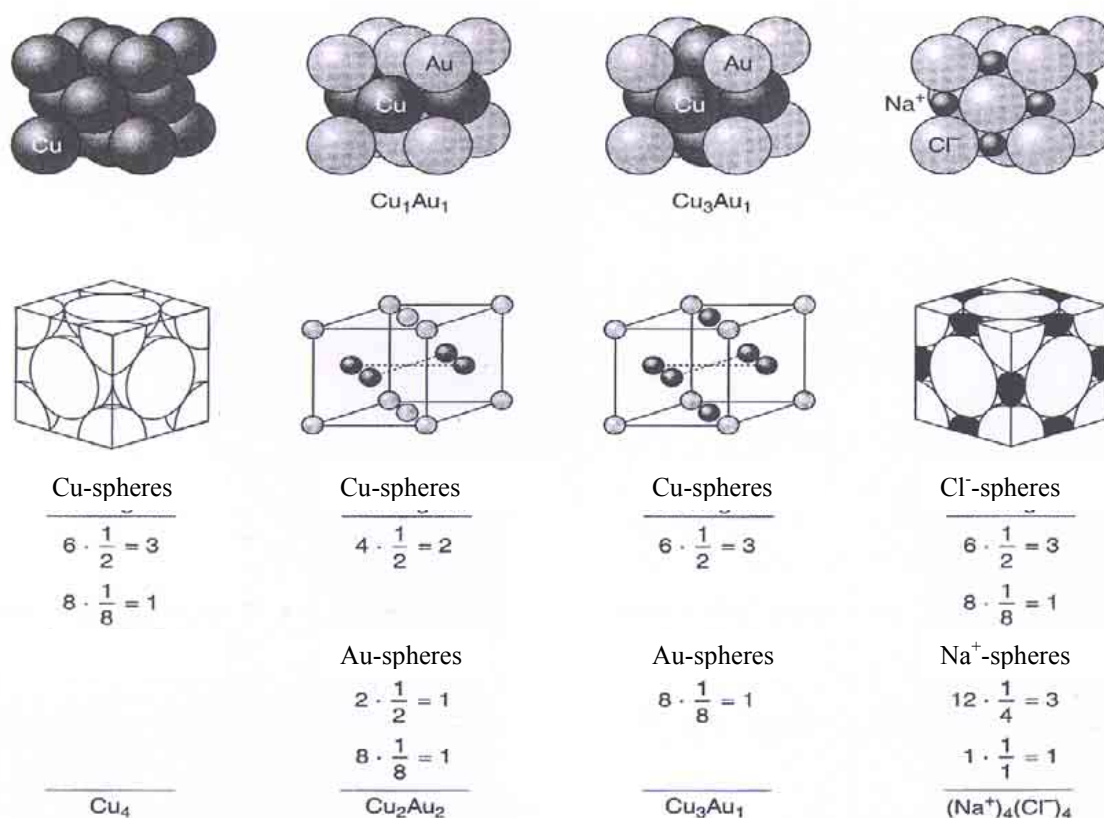
**FIGURE 6:** Face-centred cubic packings of superstructures  $\text{CuAu}$  and  $\text{Cu}_3\text{Au}$ .

graph A; but when cooled down sufficiently slowly, you will get graph B, with two special minima at 25 and 50% Au atoms. Because the first composition  $\text{Cu}_3\text{Au}$  has a mass ratio of nearly 1:1, we call this special alloy 'redgold 500'; on the other hand the second composition  $\text{CuAu}$  has a mass ratio of nearly 250:750, so we call this alloy 'redgold 750'. In both cases Cu and Au atoms are arranged in a very special order (see layers of a quadratic pyramid model in Figure 6): the  $\text{CuAu}$  structure can be shown by placing layers with square pattern of Cu spheres, followed by square pattern of Au-spheres; the  $\text{Cu}_3\text{Au}$  structure can be shown by placing layers of Cu spheres, but followed by chessboard layers of Cu and Au spheres. The symmetry is also shown by elementary cubes (see Figure 6), and if you cut them into unit cells you can derive the formulae of unit cells (see Figure 7):  $\text{Cu}_2\text{Au}_2$  in the first case and  $\text{Cu}_3\text{Au}_1$  in the second case. Using this way to derive formulae, you will get  $(\text{Na}^+)_4(\text{Cl}^-)_4$  or  $\text{Na}_4\text{Cl}_4$  with regard to the unit cell of the NaCl structure (see Figure 7), and by reducing these formula you get the usual *empirical formula*  $\text{Na}_1\text{Cl}_1$  or NaCl. Showing pupils or students the structure of any crystalline substance, they may derive formulae by finding the unit cell and counting parts of the unit cell.

### UNIT CELLS AND EDUCATIONAL RESEARCH

From results of researches on spatial ability (Barke, 1993) we know that students up from grade 8 (14 years and older) are able to count parts of unit cells: more than about half of the students could do it if models of unit cells are shown such as the examples of copper and sodium chloride (see Figure 7). If unit cells are shown as lattices of  $\text{CuAu}$  and  $\text{Cu}_3\text{Au}$  (see Figure 7), the students could only reach about 25-40 % of the right answers (Barke & Engida, 2001).

We were encouraged by these results to introduce structural chemistry in grade 8 and to derive formulae from elementary cubes and their unit cells shown by full spheres or parts of them. Because of the importance of metals in every-day-life and students' knowledge of alloys like brass (household), redgold (piercing), solder (combining metals), copper-nickel (coins, nickel-allergy) or amalgam (dentist), we were very interested in teaching this topic and to show some experiments.



**FIGURE 7:** Elementary cubes and unit cells of copper,  $\text{CuAu}$ ,  $\text{Cu}_3\text{Au}$  and  $\text{NaCl}$ .

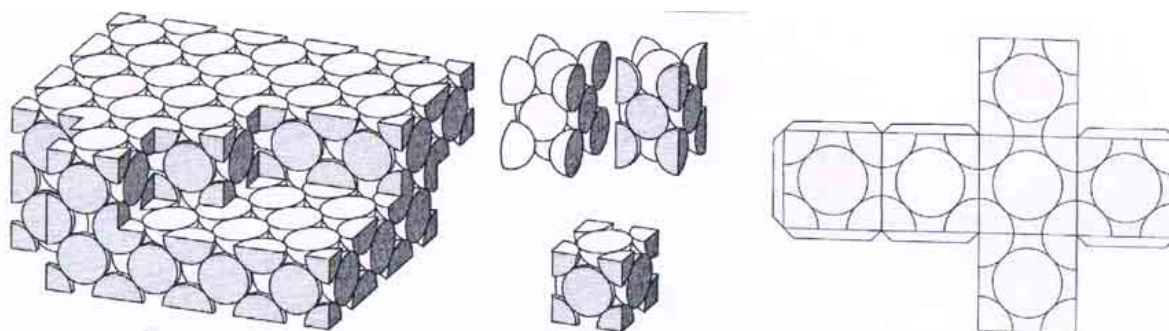
Working with copper means to combine metal atoms "left and left in PSE", to have the face-centred cubic structure, to build close packings of spheres and elementary cubes easily (see Figure 4). Taking the superstructures of the Cu-Au system means to have the opportunity to derive formulae from face-centred cubic unit cells and to show students that formulae such as  $\text{Cu}_2\text{Au}_2$  and  $\text{Cu}_3\text{Au}_1$  represent the composition of the smallest unit of structures (see Figure 7).

Reducing  $\text{Cu}_2\text{Au}_2$  to  $\text{CuAu}$  describes the way to get empirical formulae and to understand the meaning of both types of formulae. Later when working with molecules ("nonmetal atoms right and right in PSE") or with ionic lattices ("ions left and right in PSE"), students will understand the difference between molecular formulae and empirical formulae in this sense, and the difference between formulae of unit cells of salt structures (such as  $\text{Na}_4\text{Cl}_4$ ) and empirical formulae ( $\text{NaCl}$ ).

Students will gain images of the structure of metals, alloys, volatile substances and salts, they will know about smallest units of matter: unit cells in case of crystalline solid substances, molecules in case of volatile matter: "Imagination is more important than knowledge" are famous words of Albert Einstein that apply in this context!

But is it possible to teach eighth graders (14-16 years old) about metals and alloys, following the suggested way? Will they understand the significance of metal structures and formulae of alloys? Are they really happy with this kind of instruction? Our researches offer





**FIGURE 8:** *Introduction of unit cell by cut-outs of sphere packings, cardboard model of unit cell.*

some answers. Firstly we will give details about contents of the lectures, secondly hypotheses and an investigation plan.

### **Contents of the lectures**

First lectures in chemistry are given in our state in 7<sup>th</sup> grade: showing many phenomena and performing experiments in the area of states of matter, crystallisation, solution, diffusion, and providing first explanations of these phenomena with the model of small particles of matter. In 8<sup>th</sup> grade the ideas of mixtures and chemical reactions, compounds and elements are discussed, Dalton's atomic model is presented for explanation, the periodic system brings first order to the large number of elements, atomic masses and some basic principles are introduced.

At this point we start with our special periodic system (see Figure 3), with the rules for combining atoms and ions (see Table 3) and the application to metal atoms (see Table 4). Experiences of students are elicited to make some connections to everyday-life, experiments are undertaken to illustrate some alloys. Some percentages of compositions of alloys are discussed.

Spheres are introduced as models of metal atoms, sphere packings are discussed as models of metal atom arrangements in crystals of pure metals or alloys, sphere packings and elementary cubes are built by students, coordination numbers are discussed, unit cells are derived from elementary cubes. Two special copper-gold alloys are discussed as superstructures of the Cu-Au-system, formulas are derived from unit cells of these superstructures (see Figures 5 - 7).

At the end some molecule structures "right and right in PSE" are introduced and built by a molecular building set: students grasp ideas of combining some kinds of atoms and appreciate the differences between giant structures in crystals of metals and alloys and small molecules that contain only a special number of atoms. Furthermore they understand that unit cells are the smallest imaginary units of giant structures on one hand, and that molecules are the smallest units of volatile substances on the other hand. Formulas can be derived from these smallest units and can be shortened to empirical formulas, which gives only the ratio of atoms in compounds.

**TABLE 4:** Contents of lectures according to "unit cell and deriving formulae from unit cells", for grade 8 (14-16 years old). December 2000 to February 2001, total of 20 hours.

Topics	Specifications
<p><b>1.</b> <i>The periodic system of elements:</i> "atoms and ions as basic particles of matter" (Figure 3).</p>	<p>Division into metal-atoms and nonmetal atoms; introduction of ions as smallest particles of salts.</p>
<p><b>2.</b> Rules for combining atoms/ ions according to their place in the periodic system (Table 3); metal atoms "left and left in PSE".</p>	<p>First considerations on combining metal atoms: same kinds of atoms - crystals of pure metal; different kinds of atoms - crystals of alloys.</p>
<p><b>3.</b> <i>Metals and alloys:</i> collecting every-day-life experiences; experiments undertaken by students: melting zinc, dissolving copper and watching brass, forming and heating memory metal wire.</p>	<p><i>Examples:</i> gold panning, silver and copper for coins, iron for steel, aluminium for aircraft; brass, redgold, solder, amalgam, memory metal (nitinol, NiTi), etc. and their compositions.</p>
<p><b>4.</b> Sphere packings as models for the structure of copper and gold (see Figure 4); coordination number 12; elementary cube (building of packings and cubes by white cellulose spheres).</p>	<p>Introduction of names and ideas: metal, metal-structure, structural model, sphere packing, coordination number, elementary cube and fitting into packings (see Figure 4).</p>
<p><b>5.</b> Sphere packings as models of the structure of the alloy 'redgold'; building of packings with differently coloured spheres of same size.</p>	<p><i>Random</i> distribution of Cu-spheres (red) and Au-spheres (white) in a cubic close packing of spheres (tetrahedron and pyramid).</p>
<p><b>6.</b> Introduction of superstructures 'redgold 500' and 'redgold 750'; building of packings with layers of differently coloured spheres of the same size, elementary cubes (see Figure 5).</p>	<p><i>Well-ordered</i> distribution of Cu spheres (red) and Au spheres (white) in a cubic close packing of spheres (pyramids, as in Figure 5); coordination numbers of red and white spheres.</p>
<p><b>7.</b> Introduction of the unit cell by cutting it out of close cubic sphere packing (see Figure 8a); building of a model with the help of a printed cardboard (see Figure 8b).</p>	<p>Comparing the cut out of the cubic sphere packing with the cut out of an elementary cube; counting all parts of the unit cell to get four full spheres (see Figure 7, 'copper').</p>
<p><b>8.</b> Derivation of unit cells out of elementary cubes 'redgold 750' and 'redgold 500' (see 6.); formulae <math>\text{Cu}_2\text{Au}_2</math>, <math>\text{Cu}_3\text{Au}</math> (see Figure 7); building of both unit cells (see Figure 8b).</p>	<p>Students are invited to cut both elementary cubes mentally into unit cells, and to colour the self-built models of unit cells (i.e. red colour to show positions and parts of Cu atoms).</p>
<p><b>9.</b> "Right and right in PSE": combining nonmetal atoms to give first ideas of a molecule.</p>	<p>Using a molecular building set to form models of <math>\text{HCl}</math>, <math>\text{H}_2\text{O}</math>, <math>\text{NH}_3</math>, <math>\text{CH}_4</math>, <math>\text{C}_4\text{H}_{10}</math>, <math>\text{P}_4</math>, <math>\text{P}_4\text{O}_{10}</math>.</p>
<p><b>10.</b> Tests on lectures: interpreting elementary cubes and unit cells; deriving their formulas; interpreting molecular models and deriving their formulas.</p>	<p>Known examples from lectures (<math>\text{CuAu}</math>, <math>\text{Cu}_3\text{Au}</math>); new examples (<math>\text{Fe}_4\text{C}</math>, <math>\text{NiTi}</math>, <math>\text{SnAs}</math>); known examples from lectures; new examples (<math>\text{C}_2\text{H}_5\text{OH}</math>).</p>

## Hypotheses

The main aim of our empirical research was to find out to what extent students of grade 8 were able to recognise unit cells and to derive formulae from unit cells. By working successfully with unit cells and by differentiating infinite and finite structures they may develop a better understanding of chemistry than otherwise. They also may improve their spatial ability and attitudes towards chemistry. The following hypotheses were made:

1. Students accept unit cells of cubic symmetry as the smallest units of many metals and alloys, and are able to derive formulas by counting the parts of unit cells.
2. They use the periodic table for orientation: combine metal atoms as well as nonmetal atoms. With the help of structural models, differentiate between giant structures (infinite structures) and molecules (finite structures), assign adequate formulae to structural units.
3. By working with real three-dimensional models and interpreting two-dimensional pictures of models, improve their spatial ability.
4. By building and handling structural models themselves, develop better interests and positive attitudes towards chemistry.

## Investigation design

We conducted the investigation in two classes of grade 8 in the "Anne-Frank middle school" of Ibbenbueren near Muenster. Our investigation design shows all required tests and interviews (see Table 5).

Both experimental classes were first given the spatial ability test (SAT) that has previously been described and evaluated (Barke & Engida, 2001). The test was repeated at the end of the treatment (see Table 4). Control group 1 took the test after "traditional lectures" to show if differences in spatial ability existed in comparison with the experimental group which had the opportunity to improve spatial ability by building and handling real structural models and pictures of them.

Control group 2 took the SAT-test only at the end to show differences as compared to control group 1: students of control group 1 and of the experimental group knew the SAT before their treatment or traditional lectures and could recognise most items.

**TABLE 5:** Investigation design for five parallel classes of grade 8 (middle school in Germany) (SAT: spatial ability test, T: tests of knowledge before and after treatment, Q: questionnaire about interests and attitudes, I: interviews in connection with T and Q)

SAT + T <sub>before</sub>	<b>experimental group</b> (two classes) (N <sub>1</sub> = 28, N <sub>2</sub> = 26) "Building structural models"	T <sub>after 1</sub>	Q	I	SAT
SAT + T <sub>before</sub>	<b>control group 1</b> (two classes) "traditional lectures"	T <sub>after 2</sub>	Q	I	SAT
	<b>control group 2</b> (one class) "traditional lectures"		Q		SAT

There was another test before starting the treatment ( $T_{\text{before}}$ ). This test included thirteen multiple-choice questions about chemical reactions and images of particles: burning of a candle, iron plus sulphur, thermal decomposition of mercury (II) oxide, sodium plus water, hydrogen plus oxygen; note that no formulae entered this test because formulae had not yet been taught to the students.  $T_{\text{before}}$  provided information about students' knowledge before all new lectures and showed the extent of equivalence of the groups. The results of this test did not demonstrate equivalence of the groups. Even the two experimental groups had significant difference in  $T_{\text{before}}$ : for group 1, mean 52.6% (s.d. 14.2%); for group 2, mean 64.8% (s.d. 14.5%). Note also that the teachers were different.

Both tests after the treatment ( $T_{\text{after},1}$  and  $T_{\text{after},2}$ ) should demonstrate results about students' knowledge: firstly the ability to interpret formulae after working with structural models, secondly the ability to interpret formulae after traditional lectures. Note however that  $T_{\text{after},1}$  and  $T_{\text{after},2}$  included totally different questions.

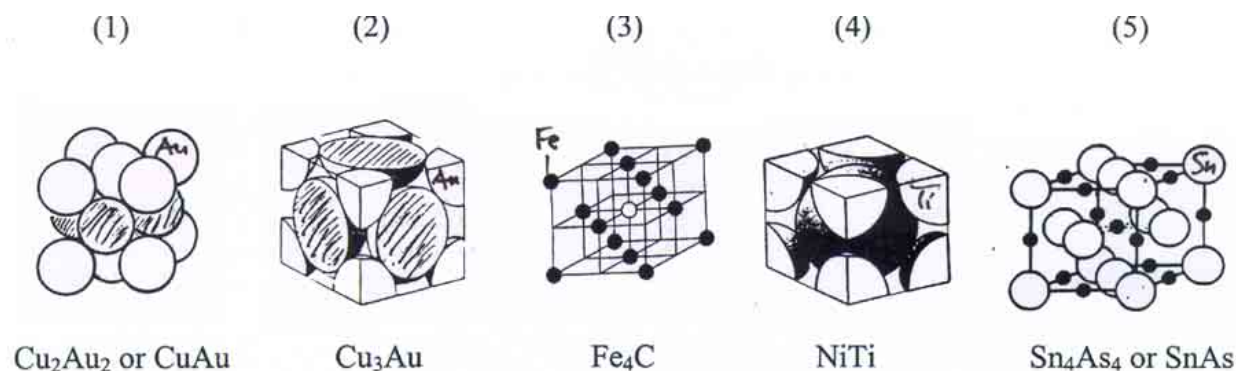
N.B. For all the above reasons (*no equivalence of groups plus the different  $T_{\text{after},1}$  and  $T_{\text{after},2}$  tests*), we will NOT report here detailed results about the performance of the control group.

The questionnaires (Q) were designed to give information about the students' interests and attitudes towards chemistry. In the interviews (I), the students of the experimental group had to give answers to open questions relevant to the treatment itself, and the test after the treatment.

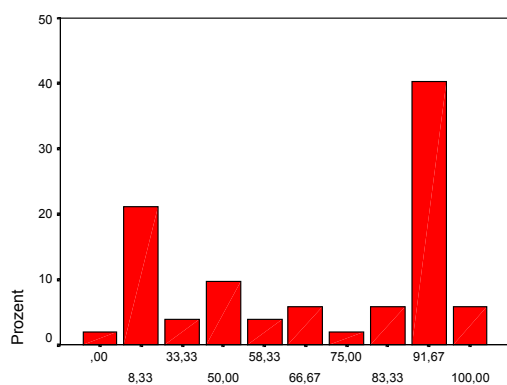
The treatment of the experimental group "building structural models" dealt with metals and alloys, with structural models like sphere packings and unit cells and formulas (see Table 4). In all control groups, teachers introduced formulae in their own traditional ways: they used the concept of valency or they compared empirical and atomic masses resulting from chemical reactions [reactions of the metal with sulphur, combustion of metals (copper or iron), and combustion of nonmetals (carbon, sulphur or phosphorus)].

## RESULTS AND COMMENTS

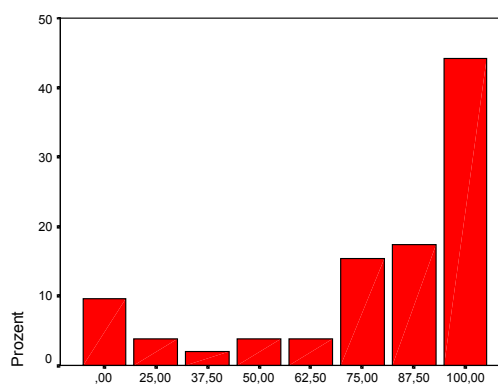
The most important information was obtained from the test taken after the treatment "building structural models" ( $T_{\text{after},1}$ ). This test contained five items and five pictures of structural models (see Figure 9). The first two pictures showed well-known structures from lectures, while the other three examples were totally new for the students. The main task for each item was the derivation of formulae. The results are shown with bar charts (see Figure 10).



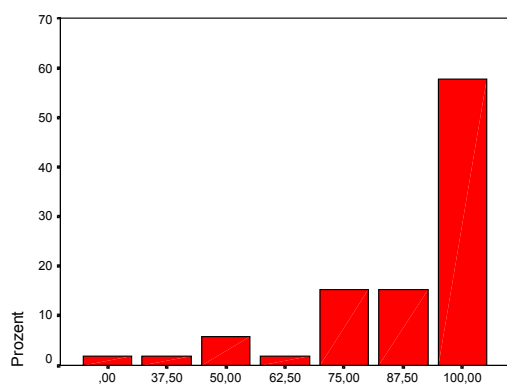
**FIGURE 9:** Pictures of structural models in the five items of the test in the experimental group.



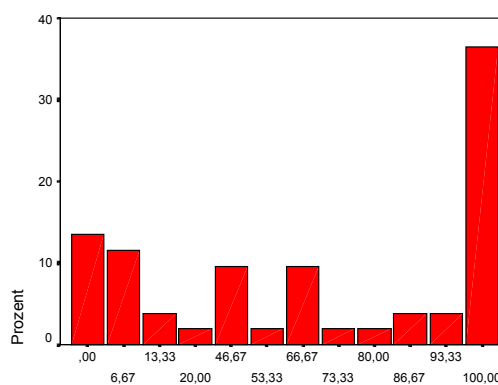
PRO1



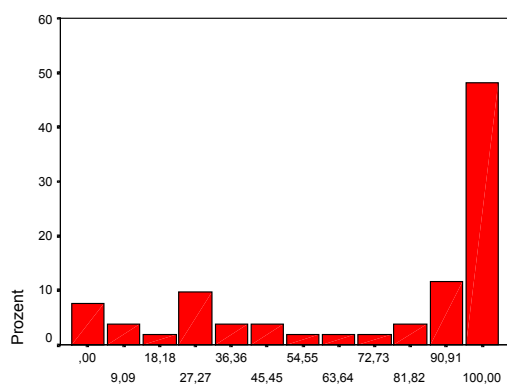
PRO4



PRO2



PRO5



PRO3

**FIGURE 10:** Percentages of correct answers in the five items of test after treatment in the experimental group (students of two classes of grade 8, middle school in Ibbenbuehren/Germany,  $N = 52$ ). [PRO 1: Item 1, PRO 2: Item 2, and so on.]

### **Hypothesis 1**

*(Students accept unit cells of cubic symmetry as the smallest units of many metals and alloys, and are able to derive formulas by counting the parts of unit cells)*

From the percentages of correct answers of the five items (see Figures 9 and 10), it is seen that more than 50 % of all experimental-group students were able to work successfully with unit cells of cubic symmetry and to find the correct formulae. The bar charts for Item 1 (in Figure 10) and Item 2 (see Figure 10, PRO 1 and PRO 2 respectively) demonstrate that it is beneficial for the students to see the parts of spheres in the picture of the unit cell (see Figure 9): while only 40-50% of the students were successful at spotting the deviation of CuAu from the elementary cube, between 60 and 70 % of them were successful with the deviation of Cu<sub>3</sub>Au from a unit cell.

Although the experimental-group students did not know structures 3-5 (see Figure 9), most of them derived successfully the unknown formulae. This data supports hypothesis 1 for more than 50% of experimental-group students in grade 8, while less than 50 % of these students did not get full marks. The following reasons can be invoked for the failures:

- careless mistakes (i.e. to add the number of full spheres instead of the parts);
- taking wrong fractions of spheres (i.e. 1/4 instead of 1/8 for spheres on corners of the cube);
- mathematical mistakes by adding fractions of spheres;
- mixing up coordination numbers and ratio formula (item 1);
- overlooking the sphere in the middle of elementary cubes (item 5).

### **Hypothesis 2**

*[Students use the periodic table for orientation: combine metal atoms as well as nonmetal atoms. With the help of structural models, differentiate between giant structures (infinite structures) and molecules (finite structures), and assign adequate formulae to structural units]*

Students of experimental classes used the special periodic table of elements (see Figure 3) and their lecture material to differentiate successfully between giant structures and molecules. Because learners of the control groups were not given any information about giant structures, they were not able to make this differentiation. The tests after the treatment (see Table 5) showed that students of the experimental group had a more profound understanding of formulae (significance of factors and indices): they correlated structural units and formulae.

### **Hypothesis 3**

*(By working with real three-dimensional models and interpreting two-dimensional pictures of models, students improve their spatial ability)*

Both the experimental and the control groups got results similar to those in other investigations of German students (Brake & Engida, 2001). In particular, most of the items that were based on pictures of cubic unit cells were solved. Students of both groups improved their spatial ability by running SAT a second time (see Table 5), but compared with students of the control group the improvement of students in experimental group was not significantly better. Therefore we cannot yet prove that handling structural models within the period of three months has a large impact on spatial ability. We assume that this impact would be significant if structural models were used over the whole period of chemical education.

#### Hypothesis 4

*(By building and handling structural models themselves, students develop better interests and positive attitudes towards chemistry)*

Analysis of questionnaires and interviews of the experimental group showed that students appreciated the handling of structural models: to work with cellulose spheres (diameter of 3.0 and 1.2 cm), to construct different sphere packings and elementary cubes (see Figures 4, 6 and 7), and the opportunity to build molecular models with the help of model sets. In particular, they liked to construct models from sweets (i.e. 'Haribo strawberries' and toothpicks). It is evident that after two or three hours of handling and discussing structural models, lectures must change to laboratory work: experiments – if possible conducted by the students – are still the most motivating activities.

### CONCLUSIONS

A meeting of about 150 persons was held some years ago in the U.S. in order to draw a list of main goals of education in science: the persons were professors from various universities, teachers from colleges and highschools, managers from industries, journalists of important newspapers. They tried to find special benchmarks for science literacy: "*Project 2061's benchmarks are statements of what all students should know or to be able to do in science, mathematics, and technology by the end of grades 2, 5, 8, and 12. The grade demarcations suggest reasonable checkpoints for estimating student progress toward the science literacy goals*" (AAAS 1993, XI).

In chapter 4 of the benchmarks "*Structure of Matter*", the authors state the importance of images of the smallest particles or of Dalton's atomic model: "*The scientific understanding of atoms and molecules requires combining two closely related ideas: all substances are composed of invisible particles, and all substances are made up of a limited number of basic ingredients, or 'elements'. These two merge into the idea that combining the particles of the basic ingredients differently leads to millions of materials with different properties*" (AAAS, 1993, p. 75).

This idea is also a central part of this paper. We offer the special periodic table of elements (see Figure 3): atoms and ions are the basic particles of matter, the combination of these basic particles will form all substances of the world. The first step means the combination of metal atoms "left and left" in the periodic table, students will know and imagine the structures of metals and some alloys. The next step should be the combination of nonmetal atoms "right and right" in the periodic table to imagine first structures of simple molecules. We could show that these steps could be realised for students in grade 8 of a middle school in Germany. This idea is mentioned also by the authors of the benchmarks: "*by the end of the 8th grade, students should know that all matter is made up of atoms, which are far too small to see directly through a microscope. The atoms of any element are alike but are different from atoms of other elements. Atoms may stick together in well-defined molecules or may be packed together in large arrays. Different arrangements of atoms into groups compose all substances*" (AAAS, 1993, p.78).

The proposed structure-oriented approach in chemical education follows the course of these "benchmarks for science literacy" and can help students to understand chemistry better than most of the traditional ways of chemical education can do. The main point should be the possibility that students can develop not only knowledge but also images by handling and

discussing structural models of matter: “Imagination is more important than knowledge” is the famous statement of Albert Einstein!

**NOTE:** All data of quantitative and qualitative analysis concerning all four hypotheses are available in the Ph.D. thesis (Wirbs, 2002) or in the *Institute of Chemistry Didactics, University of Muenster*, in Germany.

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