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THE INFLUENCE OF INTERACTIVE 3-D MODELS IN TEACHING OXIDATION NUMBERS IN ORGANIC CHEMISTRY IN THE HIGH SCHOOL CLASSROOM

MA thesis

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Abstract

Visual-spatial abilities are known to be important for all STEM learners as well as beginner-learners of Organic Chemistry since chemical concepts can only be understood if the spatial properties of molecules are clear. Thus, for this thesis, the influence of interactive 3-D models in teaching oxidation numbers in organic chemistry in the high school classroom was evaluated in a German high school. While one group was taught oxidation numbers with direct instructions on animations, the other learnt without animations in class. In a final test on both spatial ability and oxidation numbers, the learners using animations showed a tendency to outperform the other group in spatial skills with the same ability to calculate oxidation numbers. Thus, exposing students to a broad variety of visualisations might increase spatial ability which could predict better learning outcomes generally.

Keywords: spatial ability, interactive 3-D models, organic chemistry, high school

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1. Introduction

While Chemistry seems to be a very a promising field of studies since sectors such as Biochemistry, Pharmacy and Organic Chemistry are on the rise and skilled young Chemist find good opportunities to seek professional success (cf. Shwarz et al. 2021; Koerperich et al., 2020), the subject chemistry remains rather unpopular in German classrooms[1] (cf. Taimler, 2021). Even though the subject claims to explain the students' daily perception of well-known phenomena (Taimler, 2021; Pfeifer et al., 2018, Barke and Harsch, 2012), chemical concepts and given answers seem to remain not understandable for a remarkable number of students. Experiments cannot be evaluated; symbolic representations remain meaningless. That is why the subject goals cannot be met and the idea of clearing up daily phenomena turns out anything but clear for many students. As macroscopic observations, i.e. observations made with your eyes, need to be explained on sub-microscopic level, i.e. on the level of atoms and molecules, an understanding for both models and their limitations is crucially important for understanding what is said to be very logical. Thus, students with high abilities to construct mental representations of molecules can translate models more easily and therefore are superior in constructing chemical knowledge. Johnston (1993) highlights the importance of connection the levels of the visible, macroscopic level to both sub-microscopic, molecular level and symbolic level in order to fully understand chemical concepts taught in German schools

Especially in introductory classes on organic chemistry, students need to understand molecule structures in order to predict polar and non-polar bonds. A polar bond occurs when one atom has a high tendency to pull electrons while the other bond-partner has a significant lower tendency to do so. In consequence, the electrons forming the bond are shifted to one bond-partner so that a partial charge can be measured. Non-polar bonds thus occur between bond-partners with similar electron-pull so that the charge is equally distributed between both partners. The measure for the ability to pull electrons is the electronegativity. Elements with high electronegativity values pull electrons towards their core with more force than elements with low electronegativity value. As charges are responsible for the interaction of all particles, the resulting intermolecular forces, i.e. all forces between at least two molecules depend on

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[1] Taimler (2021) showed that chemistry as a school subject is either very popular for a small minority of students or very unpopular for the vast majority. Thus, students seem to either love or hate the subject with no neutral positions in between.

these electron swifts as all as probabilities for chemical reactions. That is why the skill of determining the character of a chemical bond may build the foundation for the expertise leading towards the design of new medicine or synthesis ideas if students enter the multi-layered options a chemical profession offers through these basic concepts.

However, these doors remain closed for most students who do not grasp model conceptions and fail to translate presented knowledge into correct molecule properties in their minds. Unfortunately, all ideas explained above are not visible an depend on models and the ability to create a spatial mental model. The invisible is made visible with digitalisation on the rise: Simulations, animations and 3-D models facilitate the study of the sub-microscopic level. That is why the opportunity to show students examples of how their mental representations could look like by using computer modelled 3-D molecules seems to be promising. Therefore, teachers and educators use a growing number of options to strengthen both spatial ability and representational skills. It is well known that 3-D models help students understand properties of organic chemistry (Al-Balushi and Al-Hajri, 2014), yet it is still unclear how exactly students use these models to increase their spatial understanding of molecules and contained bonds (Oliver-Hoyo and Babilonia-Rosa, 2017).

On the other hand, research on students' misconceptions started focusing on the impact of new visualisation methods, e.g. simulations or software which allows students to build their own 3-D representations on screen, too. 3-D representations are computer-modelled and allow students to look at molecules from different angles and sides while a 2-D representation can be drawn on paper. In 2-D, angles and relations to other molecules are not fully viewable, which can be seen as a limitation. On the other hand, students may also benefit from this limitation as a 3-D model is usually more complex. The Cognitive Load Theory (Mayer, 2009) states that students can only work with a limited number of information at a time. The complexity and extra information conveyed by animation or computer modelled molecules may especially be problematic for weaker students as oftentimes good to excellent students learnt best with a mixture of representational models (cf. Al-Balushi and Al-Hairi, 2014; Oliver-Hoyo and Babilonia-Rosa, 2017). Therefore, the task of conveying proper understanding of chemical core concepts remains a challenge. What exactly prohibits understanding and fosters misconceptions?

Hence, for this paper, two groups of beginner-learners of Organic Chemistry were taught the concept of oxidation numbers, i.e. numbers representing a fictional charge of atoms. In the theory of oxidational numbers, symmetrical distribution of electrons are neglected and all electrons are assigned to the bond-partner with higher electronegativity. That way, all atoms within a molecule get a negative or positive number and chemists can predict and explain reactions using these numbers. It is important to know that oxidation numbers do not necessarily represent electron density. Usually, high school students learn this concept using 2-D Lewis structures because it is easy to assign and count electrons within this structure but may lead to missing understanding of spatial properties and limitations. While one group was given classical tasks with 3-D animations as extra-studying material, the second group learnt the concept by studying the 3-D animation first and discussing its benefits and limitations in class before starting to use Lewis structures in the later stage of the unit.

As spatial ability is important for the correct understanding of molecule properties, all students took a pre-test on spatial ability as well as a pre-test in which their ability to draw basic organic components in a 2-D representation called Lewis structure was tested. After studying oxidation numbers for the same amount of time and discussing the same contexts, all students took another assessment in which they were asked to determine oxidation numbers, switch between representations and answer questions regarding electron density and swifts. The hypotheses made are

- Students learn a core concept like oxidational numbers better when introduced to it with 3-D models.
- Students need direct instructions when working with the interactive 3-D content to fully understand its limitations and benefits.

Additionally, as Mayer hints, it could be that the use of multiple representations leads to a cognitive overload. The second important set of hypotheses is

- The interactive 3-D content improves students’ overall ability to create spatial mental models.
- The extra-representation does not prohibit students’ understanding of oxidation numbers due to mental overload.

As it is still not fully understood what parameters facilitate the transfer between the different representational structures, i.e. how students increase their ability to translate spatial factors from 2-D to 3-D representation and back, answers found in this paper can be helpful for the development of future learning settings in Organic Chemistry classes on high school level. If it turns out that students benefit from additional 3-D representations when learning oxidation numbers, similar effects could be tested for other concepts, too.

2. Literature Review

2.1. Core Concepts of Organic Chemistry

Organic Chemistry is the branch of Chemistry which focuses on carbon and its special ability to build long-chained or branched molecules. Carbon has these special features because it can form so-called covalent bonds with other atoms including other carbon atoms. A covalent bond is a special bond type in which bond-partners share electrons to reach an energetically favourable state[2]. Elements vary in their ability to pull electrons towards their positively charged core. This ability is called electronegativity. Elements with a high electronegativity tend to pull electrons while electrons can be easily pulled away from elements with low electronegativity. That is why covalent bonds can be very symmetric if the difference in electronegativity is low or asymmetric if the difference is beyond a certain value. This means that in asymmetric bonds, electrons are shifted towards one bond-partner. The result is a so-called polar bond in which both partners carry a potential charge due to the imbalance of electrons. These electronic shifts in molecules due to a certain difference in electronegativity between two bonding partners have a bottleneck function for understanding concepts of Organic Chemistry (Vrabec and Proksa, 2016). Only if bonds are polar, intermolecular forces between certain molecules can be observed and only if spots with remarkably high or low electronic density can be located, certain reactions can occur since particles with a lack or surplus of electrons need a place to attack molecules. That is why properties of chemical bonds are amongst the most important teaching objectives in both school and university context. To make students understand basic ideas, the so-called valence shell model is taught to German students when they are about 13 to 14 years old. The theory states that electrons of each atom are located in different shells around the atom’s core. Electrons on the outermost shell are called valence-electrons and all elements’ tendency to fill their outermost shell with eight electrons is used to explain the majority of observations in school-Chemistry. Even though the valence shell theory has big limitations, it provides a vivid explanation and

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[2] These basic statements and explanations of Organic Chemistry can be found in any textbook on Organic Chemistry. As this paper does not aim to teach chemistry, they are limited and reduced to the amount needed to understand this paper’s reasoning.

depiction of chemical bonds: the electrons in a covalent bond are shared between bond-partners so that both partners maintain full shells. Cokelez and Dumon (2004) investigated which representations and visualisations were kept in the long-term memory of upper secondary students in France and clearly stated that the valence sphere model as well as the Lewis structures, explained in the next paragraph, are by far the most remembered.

However, many students struggle with bond concepts even in higher educational settings. As Özmen (2004) states in his review on misconceptions of chemical bonds, only a small percentage of students in various studies was able to precisely distinct between different chemical bonds. Most of them failed to explain properties of covalent bonds especially. Özmen assumes that the overuse of stick and ball models may lead to the belief that all chemical compounds are molecules. Vrabec and Proksa (2016) showed that students in the Slovakian system struggle with bond concepts, too, but identified different layers to the problem[3]. Nevertheless, they state that students tend to overuse covalent bonds and that “[t]he term electronegativity played a role in more students’ misconceptions such as confusing ionic bonding with covalent” (2014, 1368 f.), i.e. students could not translate the difference of electronegativity between bond- partners correctly to different bond characteristics. The same is true for students in German-speaking areas as highlighted by both Pfeifer et al.(2018) and Barke and Harsch (2012). While Pfeifer et al. (2018) state that the multitude of reductions in teaching due to students’ limited ability to think in abstract ways in young years prohibits learning, Barke and Harsch (2012) stress the interference of pre-concepts as students usually heard about “molecules” before their first chemistry lesson and tend to retain their oftentimes limited or incorrect preschool explanations for a long time. Either way, they agree that chemical bonds and the “clear vision are difficult to develop in school chemistry as important definitions rely on sub-microscopic, i.e. imperceptible level” (Pfeifer et al. 2018, 134) only. That is why Chemists and Chemistry teachers use a variety of iconic representations to document processes on the imperceptible level, which needs to be learnt and understood by beginners of Organic Chemistry, too (cf. Cortes et al. 2019). In addition to classical 2-D representations drawn on paper, students nowadays can also be exposed to 3-D representations in multimedia-learning settings. That is why it is important to look at multimedia learning next.

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[3] Cf. Vrabec and Proksa (2016). They discussed various factors and agents in the Slovakian Educational system not interesting for the purpose of this paper.

2.2. Multimedia Theory and its benefits for Chemistry Learners

2.2.1 Mayer's Cognitive Load Theory

Oftentimes, multimedia is linked to the use of digital devices only. This is an insufficient definition because *multi media* literally translates to *many carriers*, i.e. many tools or objects to transport a message or piece of information. That is why the definition used by Mayer (2009) understands multimedia learning in a broader way:

"Multimedia learning occurs when people build mental representations from words (such as spoken text or printed text) and pictures (such as illustrations, photos, animation, or video)." (Mayer 2009, 2)

Thus, computer-based learning can be multimedia learning – but is does not have to be, while on the other hand, almost every lesson is a multimedia setting as long as a teacher talks and simultaneously provides visual scaffolding as well. Since Chemistry learning involves a lot of models and imagination of invisible processes, technical progress allows teachers to depict the invisible by using animations, simulations or visualisations of modelling processes. Due to Pfeifer et al. (2018) chemistry is the one subject that cannot replace computer-based learning material because neither molecules, atoms or reactions can be observed directly. Hence, methods such as molecule modelling, simulating reactions or depicting electron density surfaces in 3D play an important role in modern Chemistry teaching and will continue to help students understand the invisible level.

However, according to Mayer multimedia offers many opportunities because "people learn more deeply from words and pictures than from words alone [but] (…) simply adding pictures to words does not guarantee an improvement in learning" (2009, 31). This implements that there are certain factors and conditions which prohibit learning processes in multimedia learning settings while other foster positive effects. Mayer stresses that multimedia instructions need to be designed in a way that is beneficial for human learning. In his *Cognitive Theory of Multimedia Learning*[4], he assumes that humans

- use duals channel for processing information, i.e. visually and auditorily presented information are entering the human's brain on different paths.

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[4] All information on the Cognitive Theory of Multimedia Learning are taken from Mayer 2009, 33ff.

- have a limited capacity for the amount of information which can be worked with in each channel at a given time
- have to be actively process information, i.e. they need to actively structure, evaluate and select information. Thus, learning can never be passive.

At the same time, Mayer suggests that multimedia information is processed in different channels within the cognitive structures. Figure 1 shows how words and pictures are taken from sensory memory over the working memory into long-term memory if content is successfully processed and thus “learnt”.

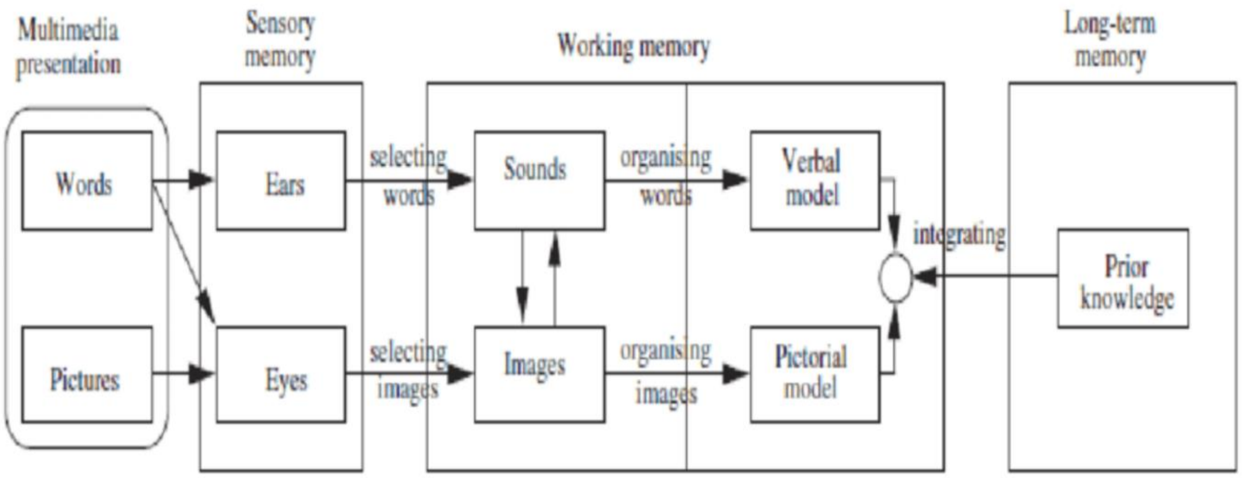

Figure 1: Cognitive Theory of Multimedia Learning (Mayer,2009, p.37)

These assumptions fit well into both core ideas of cognitivism and constructivism as the active, self-sufficient character of learning is stressed as well as cognitive processing in working and long-term memory. Trying to transfer the assumptions made by Mayer to the Chemistry classroom, one quickly stumbles across some difficulties hardly to avoid. On the one hand, students need to gain factual knowledge, i.e. theories, mathematical assumptions or terminology. At the same time, they need to achieve model competence so that they can correctly evaluate a model’s limitations and borders (cf. Pfeifer et al.,2018; Barke and Harsch, 2012). And as Chemistry often didactically reduces facts, students constantly have to alter and adapt their mental pre-models and structures. Thus, any new multimedia content may cause cognitive overload as all channels are heavily used even without presenting additional material. Hence, it is important to consider the special properties of STEM learning regarding 3-D content in addition to Mayer’s broader theory.

2.2.2 Multimedia in the Chemistry Classroom

Chemistry as a school-subject has its special properties as students do not only learn theories, but are asked to actively prepare and evaluate experiments, too. As many processes important for building up chemical understanding happen on the invisible, sub-microscopic level, multimedia content is often used to depict what cannot be seen. Kozma et al. (2000) admits that 3-D models can not provide the physical components such as smell or viscosity that the physical components can offer, but “representations play a particularly important role (…) because they enable the consideration and discussion of objects and processes” (Kozma et al., 2000, 122). At the same time, Kozma et al.(2000a) found out that chemistry students rarely used visual representations in the lab setting while experts constantly produce visual guidance to facilitate their processing of experiments and theoretical assumptions. Their ability to discuss results remained very low and could be improved by the use of modelled molecules as well as simulations.

At the same time, major findings of Mayer’s Cognitive Load Theory are true for the implementation of multimedia content in Chemistry Learning. Russell and Kozman (2009) summarize that since students learn best when allowed to interact with either physical or virtual material, a lot more research needs to be done on multimedia learning in the Chemistry classroom as major questions are rather purely understood. They suggest studying the influence of static pictures vs. animations or the study of single atoms/molecules vs. the study of entire reactions or systems. The same is true for the study of the “Representational Competence: a set of skills and practices that allow a person to use a variety of representations, singly and together, to think about, communicate (…) physical entities, such as molecules and their reactions” (Kozman et al., 2000, 105).

In conclusion, learning Chemistry can always be seen as a multimedia learning process since learners are constantly challenged on multiple channels. For this thesis, it is interesting to focus on the ability to transfer spatial properties to mental models as it is known that students with high spatial ability perform better in STEM areas like Chemistry (cf. Oliver-Hoyo and Babilonia-Rosa, 2017; Cokelez and Dumon, 2004; Wu and Shah, 2002). The representation most popular remains the so-called Lewis structure: a 2-D representation showing elements symbols and either dots or dashes to represent electro bonds. Its simplicity on the one hand might be the reason for its dominant position in the German chemistry classroom, but its probably underestimated difficulties for students on the other hand make it an interesting topic for further investigation.

2.3 Lewis Structures and Misconceptions

The most used representation in Organic Chemistry is the so-called Lewis structure[5]. In this 2-D structure, atoms are represented with the letter shown in the periodic table of elements while the covalent bonds are indicated with lines linking the letters wherever a covalent bond is located. Each line represents two electrons, one from each bond partner. The resulting structural formula are easy to draw and seem to be easy to read as well. [6] As a rule of thumb, students usually learn that all elements seek to get hold of eight electrons in their outer sphere as this represented an energetically very favourable state (cf.;Peters, 2019; Bee et al.,2019¸ Schulte-Coerne, 2014)[7].

While Lewis structures are the only representation mandatory to be taught according to German Gymnasium[8] standards (Nds. KM, 2017), much research has been done on misconceptions of standard Lewis structures as students seem to misinterpret these structures on a regular basis. A study made by Cooper et al. (2010) showed that most students of Chemistry nor Organic Chemistry in a US-American university were not capable of correctly drawing basic Lewis structures. As Cooper et al.(2010) showed, almost no student was able to correctly explain the importance of Lewis structures either. While most said they tried to follow the octet rule because “elements wanted octets” (Cooper et al.2010, 871), they were not able to explain reasons. Surprisingly, only 31% of all Organic Chemistry students correctly mentioned that chemical information can be taken from Lewis structures. Thus, they scored significantly lower than students of general Chemistry (56%), which stresses the argument that Lewis structures are probably not well understood even by Chemistry students. Cooper et al. suggest teachers to introduce concepts such as bond characters and charges before introducing Lewis structures as students need “recognition that Lewis structures are two-dimensional “short-hand” for three-dimensional information (Cooper et al. 2010, 872). That is why Lewis structures should not be shown before students have fully grasped properties of the real, three-dimensional molecules, i.e. students need to understand bond

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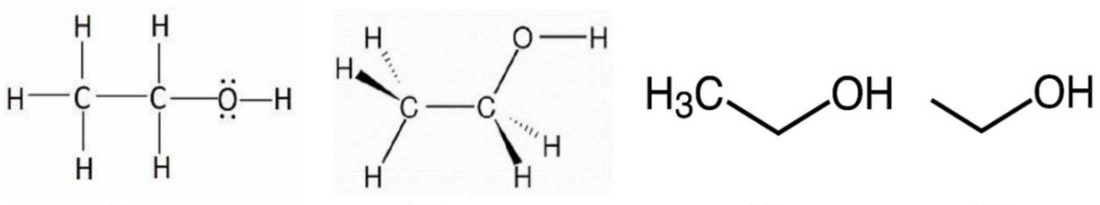
[5] It is the only representation mandatory in German schools for this reason.

[6] Examples of some basic Lewis structures can be studied in the Appendix of this paper.

[7] This again is a reductive description. Many molecules and their structures cannot be explained with this rule only. But as other factors are too complex to be taught in schools, it is still used as a standard in the German school context.

[8] I.e. the high school-like type of school, providing highest education on secondary level in the German school system. Students in Gymnasium are 10 to 19 years old and usually start learning Chemistry when they are about 13 to 14 years old.

length, electronic distribution, bond angles and intramolecular forces before they can be asked to read or draw Lewis structures as the two-dimensional structure limits the understanding of all properties based on spatial factors. This makes sense when looking at the broad variety of commonly used Lewis structures. Figure 2 shows four examples of Lewis structures of the ethanol molecule.



(1) (2) (3) (4)

Figure 2: Commonly used Lewis structures in Chemistry textbooks (cf.;Peters, 2019; Bee et al.,2019¸ Schulte-Coerne, 2014)

While depiction (1) and (2) show all atoms in the molecule, depiction (3) and (4) do not directly show neither all carbon and hydrogen atoms. Cortes et al. (2019, 15f.) showed that on average, there are about 80 different ways of representing molecules and chemical content in introductory material of Biochemistry textbooks. Due to Cortes et al. (2019) it is often not reflected that experts of Chemistry easily transfer between different representations, but expert-educators often fail to explain the differences and limitations to novice learners. The fact that mathematical and symbolic representations are not yet included shows how complicated it is to show beginners how to deal and structure all visual information (Cortes et al. 2019, 16ff.). Karonen et al. (2021) recently showed that models in themselves may hinder students in understanding new models of misconception caused by simplified structures are not yet understood. Thus, Karonen et al. highlight the importance to teach every representation with enough care for model competences (Karonen et al., 2021, 21).

High school learners are at the very beginning of their academic career. That is why the suggestion made by Cooper et al. (2010, 873) to limit Lewis structures to first and second row elements is met by the German curriculum (2017) and implemented in all commonly used textbooks, too (cf.;Peters, 2019; Bee et al.,2019¸ Schulte-Coerne, 2014). However, Lewis structures remain a struggle for many students as could be shown by Enawaty and Sartika (2015) who stress that students are more trying to find Lewis structures than thinking about the truths of chemical concepts. In this way, the Lewis structure may prohibit deep understanding. Instead of learning chemistry, students tend to learn how to satisfy the teacher’s wish to produce non-understood Lewis structures – a state that cannot be favoured by any good and responsible educator.

Providing an alternative path of teaching, Shustermann and Shustermann (1997) highlight the importance of electronic density and suggest focussing on teaching electronic density instead of Lewis structures to foster comprehension of chemical bonds. Since knowledge of bond concepts is the foundation for further knowledge building in Chemistry (Özmen, 1997; Vrabec and Proska, 2014; Shustermann and Shustermann, 1997), additional material and representations are needed to successfully teach students how electronegativity affects bond character, angle and the structure of molecules. Whether Lewis structures need to be better introduced before concepts of electronegativity or bond characteristics are introduced or whether it is better to not talk about the 2-D structure before the concepts mentioned are understood in all their spatial levels needs to be studied still. Thus, visual-spatial ability is stressed another time and proves to be a core factor for successful Chemistry learning and teaching. Hence, it is the last chapter and probably most important chapter of this theoretical overview.

2.4. Spatial Ability and 3D representations

The German curriculum for the so called “Sekundarstufe 1”, i.e. grades 5 to 10 in German “Gymnasium” or “Gesamtschule”, the two most common forms of secondary schools in the state of Lower-Saxony requires the introduction of Lewis structures in year 8. That is why students reaching 11th grade are used to representing molecules in 2-D Lewis structures already while no other representation is mandatory for organic compounds. However, many concepts usually taught and explained with Lewis structures are based on spatial factors. That is why it is questionable whether students correctly understand main issues while studying a 2-D representation or whether they can transfer their knowledge on 3-D models, too. In addition, Cooper et al. (2010) argue that many students do not fully understand all properties of the Lewis structure. Thus, research on best ways to teach Organic chemistry started to look at computer-based methods such as molecule-modelling about three decades ago. Johnstone (1993) stated that it is crucially important to link the imperceptible level to visual representations in order to successfully teach Chemistry to youth.

Today, it is known that both spatial ability and the ability to switch in between different representations is correlated to students’ grades in Chemistry classes on high-school level and early semesters in university (cf. Oliver-Hoyo and Babilonia-Rosa, 2017). In order to better test students’ abilities, Wu and Shah (2002) mention the Purdue Visualization of Rotations Test (PVRT) as well as other, non-science related tests and showed that spatial ability highly correlated with science learning success. But as the items in these tests do not ask for any chemical knowledge, it can only be concluded that the ability to mentally rotate objects helps students in learning chemical concepts. It also seems important to be capable of performing mental spatial manipulation to objects in order to do the same with presented molecule representations. As it is agreed that translation between different representations is important to gain a full insight on as many aspects of the molecule as possible, Al-Balushi and Al-Hajrib (2014) designed an “Organic Chemistry Visualisation Test (OCVT)” which was administered at the end of their study. The test can be used to examine different skills which are frequently taught in beginners’ classes of Organic chemistry. Students who are capable of mentally rotating molecules seem to have an advantage over peers who cannot manipulate mental models as easily. In addition, Hornbuckle (2014) showed that students’ ability to interpret molecules in their spatial properties were superior in solving tasks in general chemistry – students who could not imagine sub-microscopic processes failed to improve on the other hand.

That is why physical models and visualisations of the invisible structures have become fundamental instruments to help students shape, evaluate and reflect their personal, mental constructions which shall help them answer chemical questions. Hence, researchers commonly agree that 2-D representation offered by Lewis structures needs to be accompanied and supported by other representations. Vrabec and Proksa (2014) state that “teachers should use simulations, analogical models, theoretical models, and concrete models to be able to describe abstract terms or realities. Apart from that, teachers should emphasize shifts between macroscopic characteristics of compounds and sub-microscopic ones “(Vrabec and Proksa, 2014, 1365). Thereby, they follow the milestone study resulting in the didactic triangle of Johnstone (2010) which argues that visible and invisible level always need to be studied in deep connection. As some students fail to build mental representations of sub-microscopic level, research is highly interested in how transfer between the levels can be facilitated. Karonen et al. (2021) on the other hand showed that students who were frequently asked to draw stick and ball models had greater difficulties in understanding more complex structures as they tended to stick to their heuristic mental model for a long time. Thus, they stress the importance to discuss limitations of models from an early age.

As in addition to macroscopic and sub-microscopic level the symbolic representations build another hurdle, Wu and Sha (2004) concluded that the difficulties of students in transferring spatial information between different molecule depictions could be met by focusing on macroscopic instead of symbolic level. These contradicts the hypothesis of Johnstone (1993) to link the three different levels of representation as often as possible. But Wu and Sha themselves add that many students would probably stick to pre-scientific beliefs and explanations on macroscopic level as sub-microscopic and symbolic terms are abstract. Thus, Wu and Sha conclude that spatial ability needs to be trained so that students increase their ability to comprehend, evaluate and choose between various existing molecule representations in order to improve their overall chemical learning skills. As the 2-D Lewis structures represent content on a rather symbolic level, Purser's (2010) remark, that Lewis structures are meant to explain molecule structures, but neither bond quality nor electron distribution, it seems reasonable to replace at least portions of Lewis structures with interactive 3-D content to increase students' awareness for spatial factors.

As spatial ability is low for some students, scaffolding is commonly used in the Chemistry classroom to help students find a mental representation for the invisible. Pfeifer et al. (2018) list

- concrete physical models that students can put together using their hands. Physical models can be rotated and viewed from any perspective as they are "real" in the sense that they belong to the three-dimensional room.
- computer-modelled molecules, i.e. virtual 3-D models of molecules that can be rotated and manipulated on screen. Some modelling software allows students to alter the given molecules, too.
- computer-made simulations which show certain processes and aspects. Simulations can show either virtual 3-D models or other molecule representations. While virtual 3-D models can be manipulated, a simulation usually shows an entire process. Hence, alterations are limited (e.g. speed, angle or molecule in focus)

While research has been able to show that concrete physical models significantly improve spatial abilities and the ability to switch between different representations of organic molecules (Stull et al. 2012), less is known about the effects of computer-based simulations and virtual 3D models. Appling (2004) showed that software-based modelling increased students’ ability to wander between different molecule representations and improved their own 3-D models significantly but failed to prove that 3-D models helped to improve the ability to set up correct concrete models. Aldahmash and Abraham (2009)showed that students gained more understanding for a chemical reaction if they saw a kinetic instead of a static visualisation. Al-Balushi and Al-Harjib (2014) proved the mixture of concrete models and simulations superior to the usage of physical models only, but admit that simulations “enhance concrete models”, but cannot replace them. Therefore, students still need the concrete model and use the software apparently to better understand another model of the “real molecule”.Thus, it is not clear whether students correctly understand all properties of the simulations. Abraham et al. (2009) showed that especially students with higher spatial ability gained a lot of extra knowledge from 3-D animations and argued that there might be a certain baseline of spatial ability to correctly read 3-D content.

Whether and how 3D virtual models per se might help students with low spatial ability could not be solved. It is known though that general training of spatial tasks with or without chemical context helped all students to improve translation skills from 2-D to 3-D representations (cf. Hornbuckle et al., 2014). As Babilonia-Rosa and Oliver-Hoyo conclude in their review on Spatial Skills in (Bio)Chemistry education, “the causes and effects of such training [i.e. spatial training] in biochemistry and chemistry education remain poorly understood” (2017, 1003). Stieff (2020) highlights that visual chunking helps students to better spot rotated molecules as they can use colour codes to understand the changes made. But Rau (2018) adds that students need frequent exposure to colour codes to successfully translate them into spatial information.

How these strategies can be best supported by instruction remain another challenge. While Yang showed that animations with narrations are superior to animations without any explanation offered (2003), Al Balushi and Al Hajrib (2014) assigned students’ success when working with animations to the fact that they could rotate, rebuild and switch between representations of more than 50 different molecules, but failed to show that the animations themselves were responsible for the effect as students also used physical models, too. In addition to these uncertainties, there are also many ways to implement 3-D models into the classroom setting. While Yang (2003) let students work with animations on their own, Al Balushi and Al Hajrib (2014) used their animations and simulations throughout different units of teaching Organic Chemistry and asked teachers to strictly stick to a given manual. That is why the different results may also be influenced by the methods used during the teaching phases. Few is certainly known on the exact properties and mental processes which help students when working with simulations. That is why Babilonia-Rosa and Oliver-Hoyo (2017) hope that future research may focus on distinct factors to help educators understand in which way simulations and 3-D models might be used to help students understand both Lewis structures and underlying electronic density as both are keys to a full understanding of Chemical bonds.

2.5. Implementations for the Design of Material and Instructions

While many questions on spatial ability cannot be answered due to a lack of basic research (cf. chapters 2.1 to 2.4), both researchers in general multimedia learning as well as researchers in the field of teaching Chemistry agree that students understand Chemistry better certain abilities are gained:

- Mayer (2009) and Kozmann (2000, 2000a) stated that multimedia learning should be interactive so that students can manipulate factors such as speed or narration. Al-Balushi and Al-Hajrib (2014) proved that students who are capable of mentally rotating molecules perform better than students who cannot mentally manipulate molecule models. That is why it seems to be reasonable to make sure that students are always allowed to rotate 3-D models and switch between different angles of perspective. This should be helpful since students with lower spatial ability can make up for a lack of spatial ability using 3-D models.

- Spatial ability and the ability to transfer between representations do foster chemical understanding. At the same time, students benefit from spatial exercise on chemical topics as they improve by discussing and questioning experimental results on a deeper level if visual-spatial aid is given. Thus, it makes sense to not only train spatial thinking as a single entity, but to connect tasks and exercises with chemical content.

3. Methodology

3.1 Type of Research and Design

The research of this paper aimed to compare instructional methods between two groups. Data analysis methods were mostly quantitative as performance scores were collected and analysed. Parts of the analysis were qualitative as commonly made mistakes were collected and compared between groups to make up for small datasets. The performance in tests on spatial ability (dependent variable) was investigated using a quasi experimental design. While one group learnt a new concept on 3-D molecule animations in class, the control group learnt the same concept on 2-D representations. Thus, the independent variable was the type of instruction and the material included. The roles of experimental group and control were assigned to students according to their formal classes, 11b and 11e. That is why the research is quasi-experimental since the groups are not randomly put together. An experimental setting could not be organised due to both Covid restrictions and organisational issues within the school setting: This year's teaching was conducted under special circumstances due to the international Covid crisis. Thus, set classes could not be mixed for the entire schoolyear and timetables differed between classes. Hence, a randomised data collection was impossible to organise and the reason why the inferior quasi-experimental setting was chosen.

After revising basics from previous years, all students took a test on spatial ability and Lewis structures. They were introduced to concepts of electronic swift, electronegativity and oxidation numbers[9] afterwards. While in class 11b students were provided 3D animations of eight molecules to study whenever they wanted throughout all lessons, they learnt the concept of oxidational numbers with focus on Lewis structures. They first calculated the numbers by distribution of electrons in the 2-D structure and then described the importance in everyday-life contexts. 11e learnt the same concept but studied the 3-D animations in class. They were given direct instructions which included work on the 3-D molecules and learnt about oxidational numbers on the 3D structure. They discussed the same contexts afterwards. 11e was never directly asked to calculate oxidation numbers using Lewis structures, but were neither directly told not to use 2D structure. The same way, 11b was never told to not use the animations for help whenever they wanted to.

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[9] For a quick explanation of chemical terms you may have a look at the Appendix

3.2 Population

Research focused on Chemistry students in 11th grade of the German school system under the rules and regulations of the Federal State of Lower-Saxony. This means that all students in the population are aged 17 to 18 years and visit a “Gymnasium”, i.e. the German type of high school which offers highest level secondary education. As graduation from Gymnasium directly qualifies for university, it is the most popular type of high school throughout Germany. Students start education in Chemistry in grade 7, which means that they all have been taught Chemistry for four years once they enter grade 11 and start into their fifth year. About 80% of the students speak only German with their families at home and come from slightly above average social strata. The distribution between genders is almost equal with a slight majority of females. All students voluntarily decide to continue with Chemistry in the last three years which are meant to prepare them for the German A-levels. Thus, they have to take a course on Introduction of Organic Chemistry and need to learn about molecule structures and resulting behaviour of organic compounds. While some students decide to take chemistry out of personal interest and delight, others take chemistry to avoid another STEM class as all students have to take three out of four classes in Biology/Physics/Informatics and Chemistry. In my school, a total number of 5 courses in Chemistry is offered each year. Two of these courses (11b and 11e) were asked to participate in the research and stayed together in their classes

3.3 Sample and Sampling

The sample examined consists if two regular “Gymnasium” classes, 11b and 11e. They all visit the same Gymnasium in the state of Lower-Saxony, Germany and were chosen because they were

- accessible as the researcher personally teaches both groups
- just started the introductory phase of the German A-levels, which means they all started courses this year and should not differ in pre-knowledge
- are representative of the population in terms of social strata and gender
- chose Chemistry on a voluntarily basis
- grouped together in classes of similar size so that they can be compared to each other in a quasi-experimental setting

Class 11b is a so-called tablet class, which means that all students work with a self-owned tablet throughout all lessons. Students of the school can decide whether they want to be in a tablet-class after year 10. Since the tablet-classes are very popular with the students, class 11b is slightly bigger than class 11e. There were 22 students in 11b at the beginning of the schoolyear, one student decided to drop chemistry after the first term. One student in 11b is non-German native speaker and struggles a lot with both language and academic requirements. There are 19 students in 11e. All of them continued the Chemistry class after the first semester. That is why there are in total 21 students in 11b (N_1) and 19 students in 11e (N_2) who participated (N_{total}=40) in at least two out of three tests. 9 students (=S_1) out of N_1 and 7 students (=S_2) out of N_2 finished all tests. There was one final assessment which was not taken into consideration as notes on the tasks were indicated in both English and Arabic suggesting that the student probably did not fully understand the tasks due to language problems. In addition, the third page of that particular test was identical to another student’s test.

While at first it was planned to investigate the results of all students in 11b and 11e, a special focus was finally put on the small subgroups who performed all tests given. The initial idea to select focus groups of exceptional well weak performing (above 88% or below 45% in pre-test on spatial ability) students had to be rejected due to the small sample number of S_1= 9 for 11b and S_2= 8 for 11e of complete data sets. All students took all tests anonymously. They all chose a nickname and used that name to complete all three tests. That way, the results of individuals could be compared, but they cannot be matched with the individual student. All students were aware that the test results were used for research purposes and participated voluntarily.

3.4 Data Collection

3.4.1 Tests

All students were asked to takes three assignments in total. In mid-November, they completed a pre-test on spatial ability and isomeric structures (Test1); in April of the following year, they were asked to draw Lewis structures of nine commonly used organic compounds (Test2) and they all were all asked to complete the final assignment on oxidation numbers and 3D representations in the beginning of May. As mentioned above, only 9 students in 11b and 7 students in 11 e finished all three tests. Test 1 was written in class with a very broad time limit so that students did not feel pressure. 19 students were present in 11b the day the test was taken; 17 students were present in 11e. All missing students uploaded the test results to the school's Learning Management System so that data from the total number of N_1/N_2 could be collected.

The test on Lewis structures asked for nine structures. The sample compounds were identical to the ones used by Cooper (2010) to show that high school and university students struggled with Lewis structures. The purpose was again to prove whether the same assumption was true for both groups before they started the teaching unit on oxidation numbers. Additionally, both pre-tests were meant to make sure that both groups were comparable to diminish the weakness of the quasi-experimental setting. The task on Lewis structures was a homework assignment during a lockdown phase. The final assessment was also given as homework assignment after completion of the teaching unit on oxidation numbers. Items asked for oxidation numbers, electron density and the transfer between different representations. Hence, the scores were split into three categories representing these three areas. The entire final assessment can be studied in the Appendix of this thesis.

3.4.2 Instruments and their Validity

Test 1 consisted of three different parts: In the first part, students solved 15 items from the *Vandenberg and Kruse Mental Rotation Test* (1978). In the second part, they answered 8 items from the *Purdue Spatial Visualisation Test (1976)* and in the third part, they were asked to decide whether a pair of molecules was identical or isomeric, i.e. identical in terms of the kind and number of atoms, but different in the structural bonds. The last part consisted of 10 items, so that in total a number of 33 items was used to see whether the described correlation between spatial thinking and task on Organic Chemistry could be reproduced for both groups. The pre-test was also used to make sure that both groups were comparable and started with similar abilities into the teaching unit.

Both *Mental Rotation Test* and *Purdue Spatial Visualisation Test* are officially validated and reliable. The items on isomeric structures were taken and altered from schoolbooks (cf. Peters, 2019; Bee et al.,2019¸ Schulte-Coerne, 2014) or self-created using a molecule modelling software. Students answered questions on isomeric structures in their first classtest prior to the research questions and scored similar results in average. Thus, the tasks given are valid. The Lewis structures used in Test 2 were taken from Cooper (2010) and were thus tested in a published research study. In addition, students were not given any information on Lewis structures prior to the study. Thus, they answered the questions based on their pre-knowledge and showed similar weaknesses and mistakes in class tests before and after the assignment. Thus, the results should be valid and reliable as the structures chosen by Cooper (2010) ask for very typical abilities regarding Lewis structures.

In the final assessment, students were asked to answer a total of 9 tasks that consisted of a total of 21 items. Part of the questions directly asked for oxidation numbers (35% of scorepoints) as these were the recent focus in class; the other part focused on visual-spatial abilities (65%). Questions on visual-spatial ability can be split into two sub-categories:

- A: ability to transfer between different visual representations of molecules (43%)
- B: ability to predict chemical behaviour of components (13%)

The items were designed in reference to parts of the *Organic Chemistry Visualisation Test (*cf. Al-Balushi and Al Hajrib, 2014), but needed to be altered, changed and augmented to fit the German educational context. As many items were directly translated from the officially validated *OCVT*, especially the altered questions and the German language needed extra-validation. A test-run for the test in two courses not-involved in the experiment directly had to be cancelled due to Covid circumstances.

3.4.3 Interactive models

The interactive models used were created in Blender and show eight different organic compounds in three representations. Each representation focuses on a slightly different aspect of bond quality:

1) The molecules are shown in stick-ball model. Electrons form the “sticks” between atom- “balls”. The focus is the overall structure of the molecule.
2) The electrons form density clouds between and around each atom. Areas of high electron density are shown in red; areas of low electron density are shown in blue.
3) The bonds are in focus but are not shown as “sticks”. Instead, they form symmetrical or asymmetrical clouds in between the atoms. The focus is thus set on the swift due to electronegativity-differences.

Students can zoom, rotate or switch between the models. They can also pause, rewind or skip parts of the animation. Figure 3 shows one example of an ethanol molecule in all three visual representations.

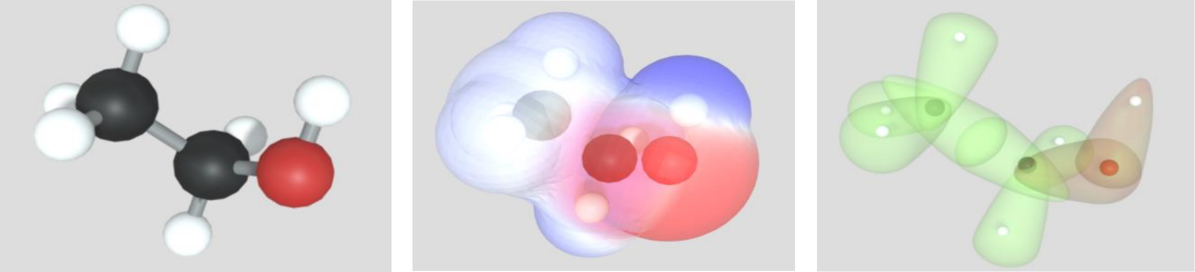

Figure 3 : Depiction of ethanole in (1) stick-ball model; (2) electron density cloud and (3), electron bond clouds. Created by Leo Siiman and available online at the platform Sketchfab, see https://bit.ly/3v607NT

3.5 Data Analysis

For both pre-test on spatial ability and final assessment average mean and standard derivation of both groups were calculated. Additionally, an independent T-test on significance $p<.05$ was done on the one-tailored hypothesis that 11e was not weaker than 11b prior treatment. Post treatment, the T test was used to assess differences between the two groups. For the post test, typical mistakes were counted for both 11b and 11e and compared, too. The t-Test was chosen and preferred against the Mann-Whitney U test because the data collected can be measured metrically.

For the test on Lewis-structures, commonly made mistakes were clustered and compared between both groups to see whether the two groups showed any significant difference prior to the teaching unit. The evaluation of mistakes was qualitative as the test-types were put into categories. The magnitude for each mistake was again quantitively examined and compared between both groups.

4. Results

4.1 Pre-and post-treatment tests/quantitative analysis

4.1.1.Results for Pre-test on Spatial ability

Table 1 presents the results of the pre-tests on Spatial ability for both 11b and 11e, showing arithmetic mean (M), standard derivation (SD), t-score and p-value for each test part and the entire test in total.

Table 1: Arithmetic mean, standard derivation and T-test parameters of 11b and 11e in the pre-test on spatial ability

Test	11b		11 e		t-score	p-value
	M	SD	M	SD		
MRT	.72	.27	.79	.17	-0.86752	.196
PSVT	.76	.20	.73	.17	0.45188	.327
Isomer-Test	.68	.11	.72	.10	-1.17647	.124
Test total	.72	.15	.76	.13	-0.75609	.227

There is no statistically significant difference between 11b (M=23.76; SD=4.98) and 11e (M=24.94; SD=4.21) in prior treatment test results. The same is true for all three test parts separately as well. Thus, the hypothesis that 11e was not weaker 11b before treatment is true and 11b and 11e are comparable.

4.2.1 Final Assessment Test

Tables 2 a and 2b present the results for the final assessment test for both 11b and 11e. While Table 2a shows the results for test sections on oxidation numbers and visual-spatial abilities, Table 2b presents the results for sub-categories of spatial ability, i.e. visual-transfer and prediction of chemical behaviour.

Table 2a: Scores for each test section of final assessment test

Part of test	11b		11e		t-score	p-value
	M	SD	M	SD		
Oxidation numbers	.73	.18	.73	.28	-0.00869	.496595
Visual-spatial ability	.59	.18	.70	.09	-1.38727	.093525

Table 2b shows the results of visual-spatial ability for 11b (M=.59; SD=.28) and 11e (M=.70; SD =.09) split into categories A and B.

Table 2b: Sub-scores in Categories A and B

	11b		11e		t-score	p-value
	M	SD	M	SD		
A: visual-transfer	.67	.19	.77	.13	-1.07903	.149408
B: prediction properties	.44	.17	.57	.17	-1.29797	.107638

There is no statistically significant difference between 11b and 11e in either ability to name oxidational numbers nor visual spatial ability with significance level $p<.05$. However, 11e scored 10% higher in average on questions on visual-spatial ability. At significance level $p<0.1$, there is a statistically significant difference between the groups compared. There is no statistically significant difference between 11b and 11e in sub-categories A nor B although 11e scored higher in both subcategories in average. There certainly is no difference between their ability to calculate oxidation numbers.

In total, there are four hypotheses as groundwork for this paper:

1) Students learn a core concept like oxidational numbers better when introduced to it with 3-D models.
2) Students need direct instructions when working with the interactive 3-D content to fully understand its limitations and benefits.
3) The interactive 3-D content improves students' overall ability to create spatial mental models.
4) The extra-representation does not prohibit students' understanding of oxidation numbers due to mental overload.

With the results given, the hypothesis that students learn the concept of oxidation numbers better when exposed to interactive 3-D content (1) is false since both groups performed almost equally well on questions on oxidation numbers. For the same reason, hypothesis 4) should be true. The hypothesis that students improve their spatial mental models seems to be true as the tendency for superior performance in the visual-representational area of 11e (M=.70; SD=.09) in comparison to 11 b (M=.59; SD=.28) is clearly visible.

4.2 Typical mistakes/qualitative analysis

4.2.1. pre-test on Lewis structures

For the pre-test on Lewis structures the most common mistakes for 11b and 11e were clustered into categories. Table 3 shows the occurrence of mistakes in 11b and 11e in percentage.

Table 3: Most commonly made mistakes in 11 b and 11 e in pre-test on Lewis structures

Type of Mistake	11 b	11 e
all structures correct	.00	.00
missing bonds	.74	.68
Violation of octet rule, i.e. atoms were given too many or two few electrons	.47	.38
Formal charges are neglected	.86	.83

Mistakes made in Lewis structures were similar in groups 11b and 11e. Both had difficulties with ionic charges within molecules and no student was capable of drawing nine correct structures. Hence, the observation made by Cooper et al. (2010) for US students seems to be true for German high-schoolers as well.

4.2.2. Mistakes made in final assessment

Mistakes or obvious misconceptions revealed in the final assessment test were clustered for both 11b and 11e. Table 4 presents the occurrence of each mistakes for 11b and 11e in comparison.

Table 4: Types of mistakes committed by students in 11b and 11e in the final assessment test

type[10]	11b	11e
Non-depicted atoms are neglected	.78	.14
C-H bond is valued polar	.33	.56
Insufficient clustering of atoms	.00	.57
Inability to spot isomeric structure indifferent visual representations	.56	.00

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[10] For samples of mistakes, see Appendix

The mistakes most commonly made in the final assessment differ between groups 11b and 11e. While some mistakes occurred frequently in 11bs' tests with no frequency in 11e, other types of mistakes are very common for students in 11e but cannot be spotted for 11b. Overall. There were particular items on spatial ability troublesome especially for 11b. At the same time, students chose different ways of representations in their results. Examples of solutions for 11b and 11e are shown in Figure 4. As presented in Figure 4a, students in 11b used the Lewis structure as basis for depictions of electronic density and structural representations while students in 11e used representations independent from the Lewis structure more often.

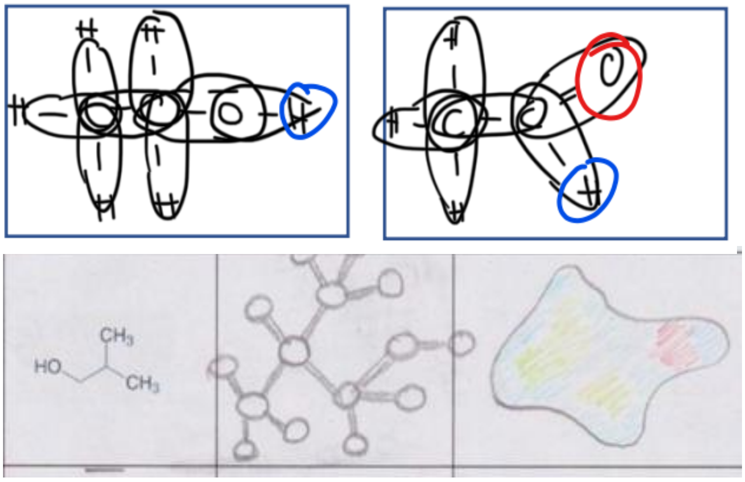


Figure 4a: variety of representations used by students in 11b (above) and 11e (below)

In addition, students in 11b failed to read reduced Lewis structures more often. Figure 4b shows the difference between 11e and 11b for one item of the test in which oxidation numbers had to be calculated for a reduced Lewis structure.

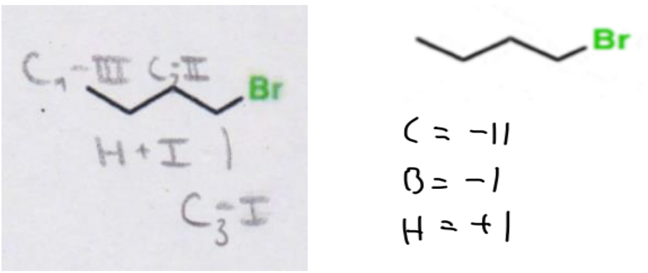


Figure 4b: students reading of reduced Lewis structure in 11e (lefthandside) and 11b (righthandside)

5. Discussion

5.1 Teaching spatial ability “to go”

On first sight, it does not seem necessary to show students interactive 3-D animations when teaching oxidation numbers as the pure calculation can be done algorithmically without having much chemical understanding. Focusing on the competence mentioned in the German curriculum (cf. Nds. Kultusministerium, 2017), both students in 11b (M=.73, SD=.18) and 11e (M=.73, SD=.28) performed equally well. As one hypothesis stated that students learning oxidation numbers with interactive 3-D content would outperform students learning only with 2-D structures, it could be concluded that the intervention was simply unsuccessful. But on second thought, students who can only calculate oxidation numbers, but not draw any deeper conclusions will not benefit much from this skill. That is why the result of oxidation numbers should rather be phrased this way: Interactive 3-D content does not prohibit learning calculating oxidation numbers while at the same time, the ability to wander between visual representations is increased.

Even though the significant difference in solving tasks in visual representations in between 11b (M=.59, SD=.18) and 11e (M=.70, SD=.09) could only be shown on significance level p<.10, the typical mistakes of both groups reveal that students in 11e most likely gained more skill in working with different representations. While they were not only able to solve more tasks in which the exercise directly asked to transfer between representational forms, about half of the students in 11e used different visualisations throughout the assignment without being ask to switch tasks. Students in 11b used the Lewis structures if not directly asked to provide other forms. Figure 5 shows typical results from 11b and 11e in comparison when asked to draw clouds of electron density.

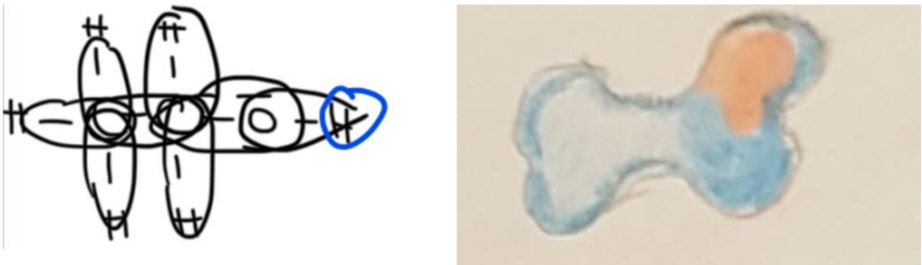


Figure 5: Electron cloud representation drawn by students in 11b (lefthandside) and 11e (righthandside)

The Lewis structure is still clearly visible for the result produced by students in 11b while the electron cloud depiction made by students in 11e is fully independent. Regarding Purser (2010) it seems as if the students in 11b use the less fitting representation as Lewis structures cannot depict electronic distribution per se. In addition, the spatial properties are better met by the result shown in 11e since the ethanol molecule is not linear and high electron density is indeed found around the red-labelled oxygen atom. Hence, students in 11e seem to outscore 11b regarding their ability to independently evaluate representations. Wu and Shah (2004) already stated that especially students with low spatial ability drew insufficient structures and thus, failed to solve questions on chemistry content. But as 11b and 11e were not significantly better in neither drawing of Lewis structures nor visual-spatial tasks, it seems likely that the interaction with the 3-D content in class helped students in 11e to improve visual spatial skills. The same is true for all tasks in which students in 11b forgot to count non-depicted carbon or hydrogen atoms when calculating oxidation numbers.

Another important factor when learning chemistry is the skill to draw, discuss and interpret limitations of different representations. Abraham (2009), Wu and Shah (2004) as well as Kozmann (2000) stated that experts in (Organic) chemistry easily switched between different representational models and were always aware of limitations in models while beginners often not understood implicit limitations. Figure 6 shows a result from a student in 11e, another student in 11e used a similar representation with no student in 11b using this limited Lewis structure.

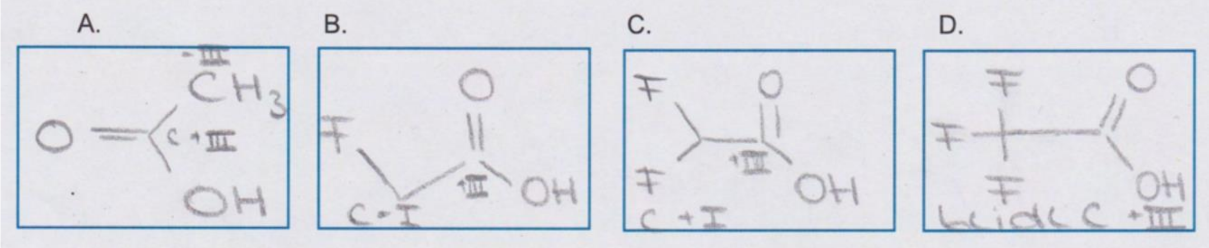


Figure 6: Students in 11e used reduced Lewis structures

While students in 11b forgot Carbon and Hydrogen atoms when not shown in the representations provided (.78 vs. .14 in 11e), almost a third of the students in 11e not only passively read limited Lewis structures, but started using them correctly, too. Pfeifer et al. (2018) state that usually novices have problems in understanding limited Lewis structures as they have to understand that the spatial properties are still met even though not shown in the limited structure. Thus, the student actively drawing a limited structure might not be seen as a novice by Pfeifer nor Wu and Shah (2004) who state that students need conceptual knowledge rather than spatial ability when actively transforming representations. As the students in 11e could not draw sufficient Lewis structures prior intervention, the fact that they had interacted with 3-D models might have helped them to fully integrate the properties such as bond number and quality into their mental visualisation skills. That could be the reason why they themselves do not see why the full depiction of all atoms should be necessary anymore. That is why common clusters of atoms (e.g. CH_3) might not be shown in structural representation either. In this case, interviewing the student could be quite fruitful to find out the true reasons for her improvement in dealing with limited 2-D structures. It could also be used to validate the assumption that the interactive 3-D content played its role in the improvement.

In addition, students in 11e correctly spotted isomeric structures in the very last question of the test while more than half of students in 11b (.59) did the same mistake which is depicted in Figure 7.

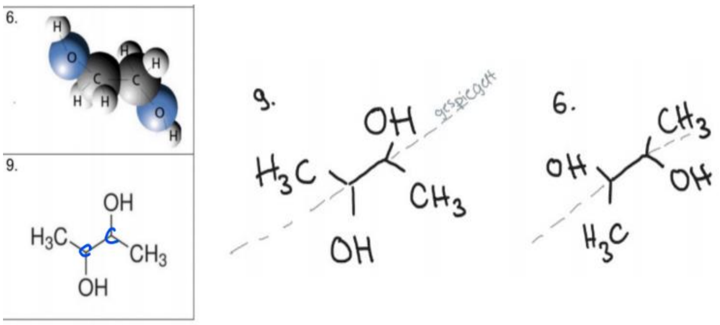


Figure 7: 59% of students in 11b considered items 6 and 9 isomeric

The blue C-atoms added by the teacher show that the students did not understand the limited structure. No student in 11e did the same mistake which again gives a hint that students in 11e might have improved their ability to read limited structures with the help of the interactive animation.

To wrap up, the major goal in curricula terms was set on oxidation numbers, students in 11e increased their visual spatial abilities (M=.70, SD=.09) with certain significance compared to 11b (M=.59, SD=.18) as a side effect – they equally met the goal of learning calculation of oxidation numbers. And even though the pure ability of transferring between visual representations in 11b (M=.67, SD=.19) and 11e (.77, SD =.13) is not significant, a well-reasoned tendency can be seen when taking into consideration the qualitative mistakes made especially in 11b. In the long run, the benefits for 11e might be more obvious as the oxidation numbers are used to predict behaviour in reactions. The ability to predict chemical behaviour was comparatively low in both 11b (M=.44, SD=.17) and 11e (M=.57, SD=.17), but with yet again a tendency in favour of 11e. Thus, the interaction with the 3-D animations seems to have had positive effects with no indication for negative side-effects. That is why it seems that 11e benefited from the interactions mostly. If similar results could be produced with bigger samples, the fear of producing cognitive overload in terms of Mayer (2009) might be groundless. This could open opportunities to train spatial skills and visio-spatial thinking alongside curricular requirements without loss for students. At the same time, students could slowly learn to break away from Lewis structures to become competent users of a broader variety of representations – an expert skill due to Wu and Shah (2004) and Kozmann (2000, 2000a). This approach could also help educators to overcome the hurdle of explaining more advanced Lewis structures which need knowledge on electron distribution and advanced atom models.

Some textbooks started to display more advanced Lewis structures, i.e. structures which try to acknowledge bond length as well as resonance effects. Badenhoop et al. (1995) used NRT methods to calculate bond lengths, bond indices and characteristics of bonds to see whether the modern structures were closer to show the “true” values within a molecule and showed that many modern Lewis structures still miss accurate depiction of important bond information. Thus, Badenhoop et al. (1995) argue that it might not be worth to confuse Chemistry beginners with Lewis structures which they cannot understand. Purser (2010) argues that Lewis structures should never contradict true electronic distribution and backs up his argument backed up by calculations based on quantum theory – a theory much superior to the valence shell theory used in German high schools. As students usually rely on Lewis structures, they have to live with reduced knowledge, which can be problematic in terms of heuristics (cf. Karonen et al., 2021), but if they were more often exposed to a broader variety of representations, there seems to be no reason for them to not understand theories focusing on electron distributions.

5.2 Spatial ability AND Lewis structure

In fact, ideas of teaching basic concepts with special focus in true electron distribution are rather old.Shustermann’s and Shustermann’s (1997) idea to teach molecule structure and electronic density before introducing any 2-D representation of molecules still seems to be a promising approach since electrons and electronegativity are the core of both, bonds in molecules and the interaction between several molecules. While in the late 1990s, it was probably still a problem to find ways and means to bring 3-D models into classrooms, students nowadays may benefit from a dual approach: They could first build physical models, study interactive 3-D models and understand bond qualities before given the 2-D Lewis structure. Purser (2010) calculated electronic density of bonds and showed that the results resemble commonly used Lewis structures so that students may be able to easily transfer between both representations. This again backs up the claims made by Shustermann and Shustermann(1997) as well as Cooper et al.(2010) to focus rather on 3-D depictions of molecules and electrons than to teach “Lewis structure and octet rule.” Figure 8 shows representations from Shustermann and Shustermann’s teaching approach as well as the density calculations by Purser (2010).

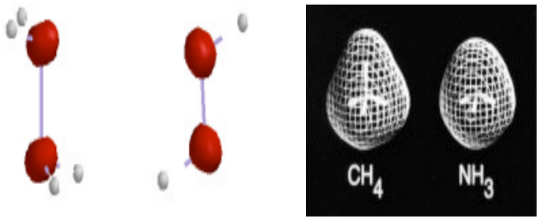


Figure 8: Density model of H_2N-NH_2 and HN=HN, Purser(2010); density models suggested by Shustermann and Shustermann (1997)

Both representational ideas resemble the Lewis structures so that students may find it easy to transfer from the familiar structures towards new modes of representations. The same was true for the interactive model used for this thesis. It might be a reason why students in 11e were surprisingly quick in decreasing their use of the full Lewis structure. The fading similarity between Lewis structure in the interactive animations is shown in Figure 9.

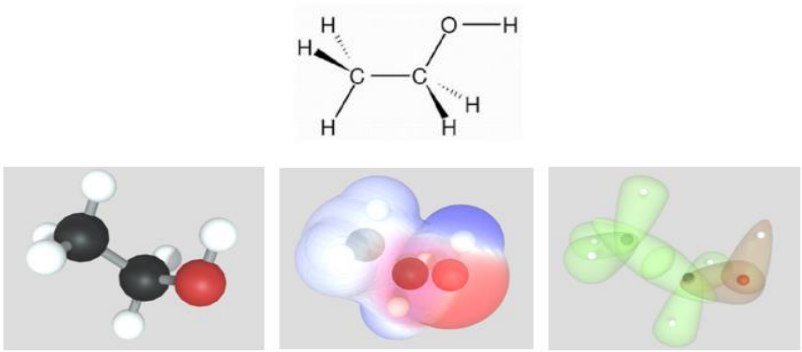
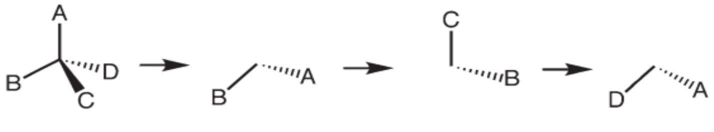


Figure 9: Parts of the interactive model in comparison to a “Lewis structure” with extra spatial information.

Nevertheless, it might also be the case that students in 11e started reproducing what they had seen in the interactive content without fully understanding these representations either. Their slight superiority in predicting chemical behaviour (M=.57, SD=.13) needs extra-validation with larger sample sizes and/or qualitative interviews. Either way, Lewis structures could be used to foster spatial understanding for all chemistry students.

5.3 Hidden potential of the Lewis-structure

The Lewis structure is extremely popular in the German chemistry classroom – oftentimes it is the only representation taught to students. Thus, it cannot be a surprise that students overuse it in contexts not appropriate. Barke and Harsch (2012) and Pfeifer (2018) admit that model competence is a core skill for chemistry learners, but Cooper (2010) adds that in the case of Lewis structures students neither know how nor why they should be able to read it. At the same time, Cortes (2019) points out the multitude of representations used, but not explained in the classroom. Thus, educators might have to use Lewis structures in a more meaningful way. Karonen (2021) adds that heuristic believes are deeply anchored in students' cognitive structures and it takes much time and effective explanation to overcome these obstacles. Interestingly, the students in 11e who scored highest and started using limited structures understood that spatial information was shortened in their representation because they still correctly calculated the oxidation numbers. While the interactive 3-D model must have helped them in a way not fully understandable, there could be other means in creating interactive models or interactive 2-D content serving the same competence. Abraham (2010) showed that students do not only need physical model kits and computer simulations to understand spatial aspects of molecules, but they also need to learn how to link the 3-D aspects to shortened 2-D representations as properties remain represented in 2-D textbooks. That is why Abraham (2010) suggests letting students solve rotation tasks similar to the MRT tasks, but on 2-D Lewis representations or Dash and wedge depictions. Figure 10 shows an item from Abrahams (2010) test.



Molecule 1 is rotated in space. Draw and complete the structures.

Figure 10: Example item for a quiz due to Abraham (2010)

Hence, interactive animations depicting classical 2-D representations that students can rotate might help enhancing their spatial abilities, too. As spatial ability as well as the skill to mentally switch between representational forms is highly correlated to successful STEM learning (cf. Wu and Shah 2004), this approach might be more helpful for students than suggestions made by Curnow (2021) to provide an altered algorithm for facilitated Lewis structures. In Curnow's (2021) approach, students need to count charges and follow rules to end up with a correct Lewis structure – an approach that focuses again on the correctness of the structure rather than on deepening students spatial skills and contradicts Karonen et el. (2021) in their attempt to decrease students' misconceptions by providing meaningful information. Their assumption that reduced knowledge may manifest pre-concepts (cf. Karonen et al.,2021) is backed by many other researchers: Abraham (2010) as well as Wu and Shah (2004) stress that oftentimes Lewis structures are introduced in textbooks way before theories on 3-D structures or stereochemistry. If chemistry educators follow this paths, they students cannot gain spatial skill unless they entered the classroom with good core-skills. That is why more opportunities should be given to students to actively interact with 3-D structures. Rau (2018) supports the claim for more frequent work with different representational forms as strategies such as visual chunking (cf. Stieff 2020) need to be internalised in the long run. Karonen et al. (2021) ask teachers to teach and focus "interrelated concepts instead of unconnected facts or using heuristics in science" (Karonen et al.,2021, 22.) so that students do not have to relearn concepts and structures over and over again. Thus, linking different representations directly to the part of depiction they are strong at while openly discussing each model*s limitation might help students a lot to increase performance in the chemistry classroom. As students in 11e worked with interactive 3-D animations for an extremely limited time only, effects could be much higher if students constantly worked with a variety of representations from the very first years of Chemistry teaching[11]. Yet again there are few previous studies focusing on young-aged students of chemistry in high-school level. Therefore, it could be a next step to introduce interactive 3-D models in grades 7 or 8 where students first learn about molecules and bond characters to see whether they could achieve better spatial skills from the very start.

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[11] Karonen et al (2021) showed that the benefits from discussing limitations of structures in class are visible after short time, too.

5.4.Open Questions on Instructions

Results from this research can be carefully read the way that students who learnt new chemical context using interactive 3-D content in the classroom increased their skill in translating representations while still getting the same ability in the newly introduced chemical concept like students who only focused on the concept, e.g. the calculation of oxidation numbers. As said above, this statement needs to be revised and used carefully, but especially with the qualitative arguments presented it seems to be a reasonable guess.

However, nothing can be said about the instructions needed for students to successfully use interactive animations in the chemistry classroom. It is questionable whether students in 11b used the opportunity to study the interactive material at all or if it was helpful for them without having the chance to quickly ask the teacher about certain properties. If they had been in the onsite classroom, they might have taken the chance to discuss what they had seen with peers and teacher, but with offsite teaching they were quite left alone. In this setting, 11b might have needed interactive animations providing more extra information. Hypervideo elements or narration (cf. Mayer 2009, Yang 2003) may improve the interactive model so that students can use it outside classroom and with less instruction needed.

For this study, the direct instruction provided to 11e cannot prove that direct instruction is superior to independent exploration of the animation as 11b might have been even better than 11e if they had used the interactive animations in class in their own pace. The popular mistakes to incorrectly value C-H bonds polar in 11e might have derived from the fact that the direct instruction stressed that the C-H bond was **not** polar which might have created special awareness for this bond type but led to a failed reading of the animation. That is why more research needs to be done to understand what type of instruction best accompanies interactive 3-D animations in class. The level of self-regulated interaction could be increased a lot as students in 11e were still exceptionally reliable on the teacher and had very low chances to manipulate the animations themselves. Thus, the full potential is certainly not understood.

In addition, the prominent mistakes of 11e give groundwork for improvement of the interactive animation, too. 57% of students in 11e clustered wrong atoms to explain their predictions on chemical behaviour – they usually put together the atoms depicted with most vivid red and blue colour in the interactive animation but failed to see that the colour code included more atoms than they thought. Stieff (2020) showed that students tend to use visual chunks when working with 3-D animated molecules. They understood both colour groups and similar size depictions as chunks and were better capable of identifying rotated molecules when visual chunks were prominent in the animation. In this case, 11e might have used a visual chunk which led to wrong conclusions. Figure 11 shows the very first part of the animation and a results from 11e in comparison.

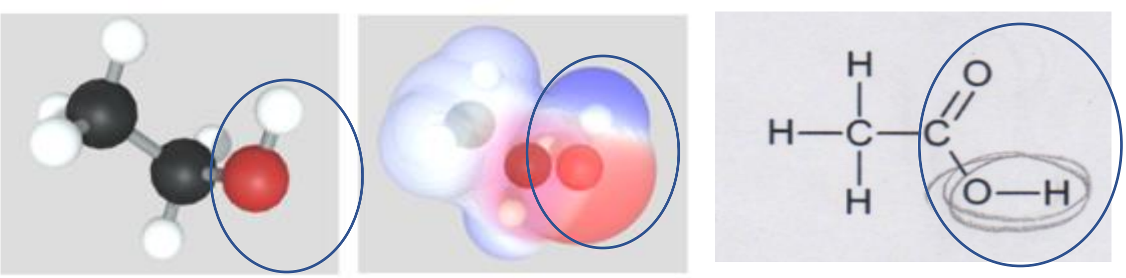

Figure 11: correct visual chunks indicated by a circle, mistake made by student in 11e

The visual chunk was not correctly transferred as the OH group is not responsible for the chemical behaviour of the component shown – the right solution would have been the blue circle shown on the right hand side. As Stieff (2020) states, visual chunks can be very helpful for students if they chunk the right portions of a molecule. They can be equally used to lead students into traps. That is why it is in interesting question whether the important atom-groups in molecules should be coloured in a way that supports chunking. Morey et al. (2015) showed that a colour redundancy facilitates change detection once the colour code is taken away. In this case, this would mean that the same atoms needed to be coloured differently as both O and H are present in the OH and COOH group. This could also lead to confusion since it would be hard for students to distinguish between sorts of atoms then. Thus, further alterations of the interactive 3-D animations could be put into the interest of further research, too.

6. Conclusion

6.1 Limitations due to Sample Size and Uncertainties due to Covid crisis

Before discussing the results and their implementations, it needs to be said that due to the small sample size all results can only be seen as a tendency. The tests needed to be redone with higher numbers of participants to be validated. In addition, the entire teaching unit is probably not comparable to any other year since the circumstances and conditions were highly influenced by the international Covid-crisis. That is why no results for hypothesis 2 can be presented and discussed, too. Students spent a lot of time in offsite teaching. Thus, their use of the interactive models was not measurable in any way. While it was formerly planned to observe when and how often 11b used the models in class when solving given tasks, it is now possible that they never looked at the models at home or that 11e also used the models while solving tasks at home. That is why especially the question on the type and amount of instruction needed to be redone in a non-Covid year.

Furthermore, students in grade 11 decide which subjects they want to continue in late spring usually. This year, organisation was different so that they already decided around Easter. As pressure was high on all students due to the unlikely situation, teaching staff agrees that this year student's motivation was incredibly low in many subjects after lockdown. Many students seem to only work for the classes they will continue next year, which may explain the low response rate for the final assessment, too. However, there might have been an effect on the entire outcome of the final assessment as it was given to students after they had decided on their future subjects. In conclusions, the results need to be seen and carefully discussed with their limitations in mind.

6.2. Implications for Teaching Organic Chemistry

Visual-spatial ability is highly agreed to be crucially important for STEM learners (Stieff 2020, Oliver-Hoyo and Babilonia-Rosa 2019, Wu and Shah 2004). That is why it should be given a prominent section within the chemical curriculum of each (German) high school. This contradicts claims and goals set in the standard curriculum of the state of lower Saxony in which spatial competences as learning objectives are fully missing (cf. Nds. Kultusministerium, 2017).

Thus, educators may have to re-think and re-evaluate the position of the prominent Lewis structure within the Chemical curricula. While some decades ago, the easy to draw 2-D representation had to be used due to lack of interactive, 3-D alternatives, it is easy to show more vivid visualisations which have fewer limitations in spatial properties than the Lewis structures to students in both high-school and university. If students were given more opportunities to work with a broader variety of representations, strategies such as visual chunking (Stieff 2020) could be easily implemented. Interactive 3-D animations could not replace but enrich the material as they offer students easy ways to improve both their conceptual skills as well as their mental rotation skills. As first suggestions to alter the school canon towards a more spatial-focus approach by Shustermann and Shustermann's (1997) concept of teaching electron density seem to have had no influence yet, single educators may have to act and use digital approaches to enlarge their teaching strategies.

While the core-curriculum directly says what must be taught in any Chemistry classroom in Lower-Saxony, it never forbids to give extra teaching so that educators have the freedom to implement as many spatial activities in their classrooms as they want. Once interactive animations are designed, they can be transferred between teachers and effectively used in many classrooms while physical concrete models can be limited or not in the inventory at all. Post Covid times might be a good time to push 3-D visualisations into more classrooms to see whether they can help students improve their spatial thinking skills alongside chemical learning. The small results made in the research presented here show that it might be worth the effort, even though general research is still growing out of kindergarten and much of grasping the invisible remains to be fully investigated and understood still.

Acknowledgements

First of all, I have to thank Leo Siiman for his help and quick work in designing animations of molecules according to my suggestions and wishes. I hope that I will be able to create similar results once I learnt more about the Blender software. Additionally, I want to thank Emanuele Bardone and the entire staff of the Educational Technology department of Tartu University for guiding us through a very “interesting” experience of a fully online, fully distant Master in incredibly special times. You made the absolute best out of it and never felt distant to me. The same is true for all my fellow students who live far away but were always close to help in times of struggles. I hope that we are going to meet each other personally in any kind of reunion once the general situation allows responsible travel again.

Author’s declaration

I hereby declare that I have written this thesis independently and that all contributions of other authors and supporters have been referenced. The thesis has been written in accordance with the requirements for graduation theses of the Institute of Education of the University of Tartu and is in compliance with good academic practices.

Göttingen, June 3rd, 2021

Ronja Dorothee Wienewski

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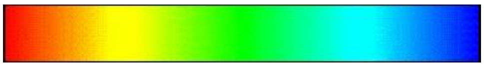
The interactive 3-D animation was created by Leo Aleksander Siiman, PhD and is available online at the platform Sketchfab, see https://bit.ly/3v607NT

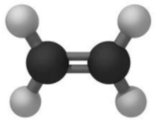
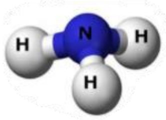
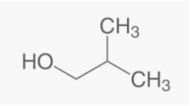
Appendix 1. Final Assessment Test in Student Version

Finaltest zum räumlichen Vorstellungsvermögen und 3D Visualisierungen

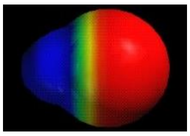
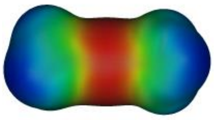
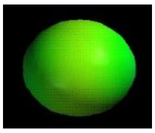
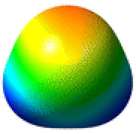
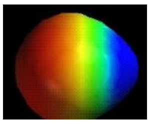
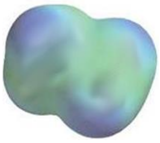
Für alle Aufgaben gilt für die Aufschlüsselung von Färbungen:



Aufgabe 1: **Ergänzen** Sie die Darstellungsformen. Achten Sie auf möglichst räumliche exakte Anordnung. **Geben** Sie die Oxidationszahlen der Atome an.

	Lewis-Formel	Ball-Stick-Modell	Elektronenwolkenmodell	Ox.zahlen
Ethanol				
				
Ammoniak				
				
Schwefel-tetrachlorid (SCl_4)				

Aufgabe 2: **Ordnen** Sie den Substanzen die korrekten van-der-Waals Elektronenwolken **zu**. (Mehrere Substanzen passen zu bestimmten Wolken).

B. C. D. E. A. F.

Substanzen: 1. HF 2. LiF 3. H_2O 4. N_2 5. H_2 6. Ethin 7. Ethan 8. LiH

Zuordnung:

Aufgabe 3: Zeichnen Sie die Lewis-Strukturformeln.

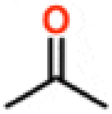
A. Ethanol B. Ethanal C. Butansäure D. 1,2-Dichlorethan

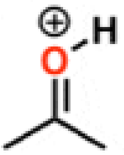
Aufgabe 4.1: Skizzieren Sie die Elektronendichte der Moleküle aus Aufgabe 3.

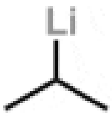
A. Ethanol B. Ethanal C. Butansäure D. 1,2-Dichlorethan

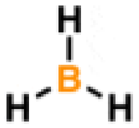
Aufgabe 4.2: Geben Sie alle Oxidationszahlen der beteiligten Atome in A.-D. an.

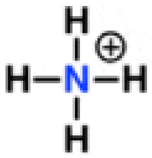
Aufgabe 5.1: Zeichnen Sie die van-der-Waals Elektronenwolken zu folgenden Strukturformeln. (Sie dürfen auch direkt „über“ die Abbildungen zeichnen.)



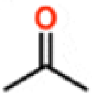


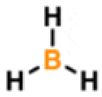


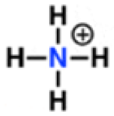


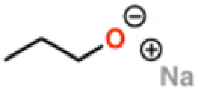


Aufgabe 5.2: Geben Sie die Oxidationszahlen aller beteiligten Atome an.







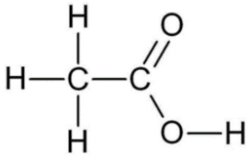


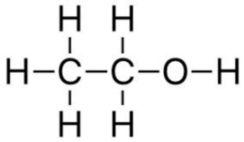
Aufgabe 5.2. **Erklären** Sie, welche der Substanzen am ehesten eine Reaktion mit einem **elektronenreichen** Bindungspartner eingehen müsste. Zeigen, wo das Molekül angegriffen werden müsste.

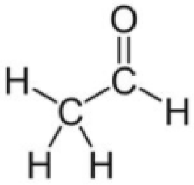
A. B . C

Reihenfolge (hohe Reaktivität – niedrige Reaktivität):

Erklärung: ____







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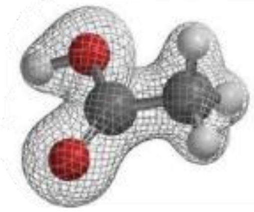
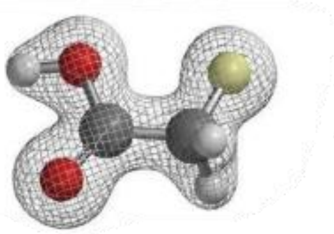
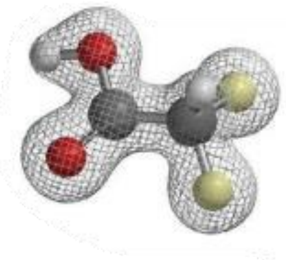
Aufgabe 6: **Zeigen** Sie anhand farblicher Markierungen die Elektronendichteverteilungen innerhalb der Moleküle (darf auf dem Papier hier passieren).

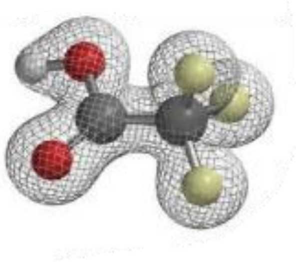
Es gilt: rot= Sauerstoff; schwarz = Kohlenstoff; weiß= Wasserstoff; gelb = Fluor

A. B. C. D.









Aufgabe 6.2: Geben Sie die Summenformeln an.

A. B. C. D.

Aufgabe 6.3: Zeichnen Sie die Lewis-Strukturen.

A. B. C. D.

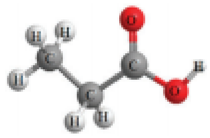
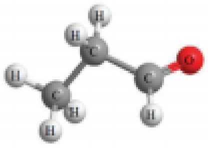
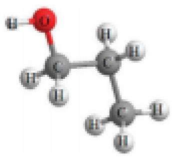
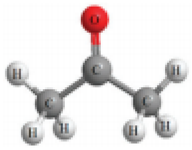
Aufgabe 6.4: **Geben** Sie die Oxidationszahlen an. Nutzen Sie die von Ihnen präferierte Darstellung und **nennen** sie diese.

Aufgabe 7: Geben Sie begründet die Substanz mit dem höchsten Siedepunkt an.

a) Ich wähle Substanz __, weil____

A. 2-Brombutan	B. 2-Brombutanol	C. 2-Brombutansäure	D. 2-Brombut-1-en

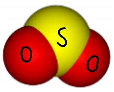
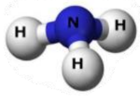
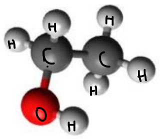
b)) Ich wähle Substanz __, weil____

A. 	B. 	C. 	D. 

c)) Ich wähle Substanz __, weil____

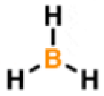
A. 	B. 	C. 	D. 

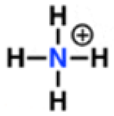
d)) Ich wähle Substanz __, weil____

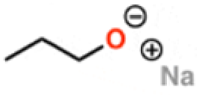
A. 	B. 	C. 	D. 

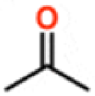
Aufgabe 8.1: Entscheiden Sie, welche der folgenden Substanzen am ehesten mit einer **Elektronenmangelverbindung** in Reaktion treten müsste. Markieren Sie die Stelle, an der der Reaktionsangriff erfolgt.

A. B. C. D. E.







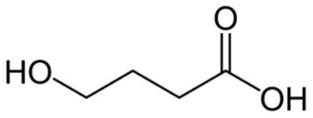
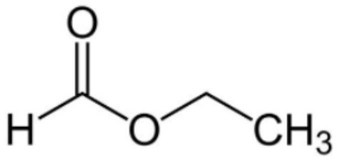
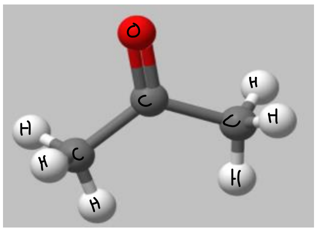
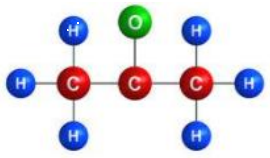
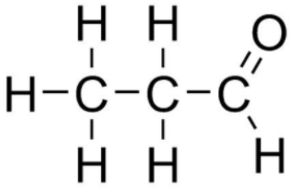
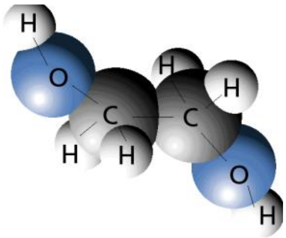
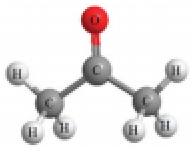
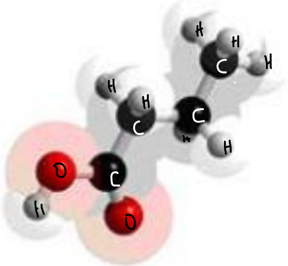
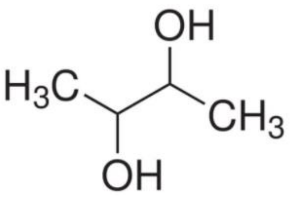


Reihenfolge (hohe Reaktivität – niedrige Reaktivität):

Aufgabe 8.2. Begründen Sie Ihre Entscheidung aus 8.1: ______________________________

____

Aufgabe 9: Betrachten Sie die Tabelle. **Entscheiden** Sie, bei welchen Substanzen es sich um Isomere oder identische Moleküle handelt. **Begründen** Sie mithilfe einer Zeichnung/Struktur.

1. 	2. 	3. 
4. 	5. 	6. 
7. 		9. 

Identisch sind ____

Begründung(en):

Isomere Strukturen sind ____

____

Begründung(en):