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Chemical Bonding: From Simple Bond Forces to Electron Pairs

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ABSTRACT

In chemistry, there are two equivalent ways of describing chemical bonding between atoms in a molecule: bond forces and electron pairs. Chemical bonding by bond forces may be introduced already in early chemistry classes – without having relations to the nucleus-shell model of atoms. Standard bonding forces can be defined easily, such as four bonds in the case of the C atom within a CH_4 molecule or two bonds in the case of the O atom within an H_2O molecule. Accordingly, proposals for chemistry education are discussed and ways of instruction are compared.

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1. INTRODUCTION

In the 1990s, our working group developed a new didactical Periodic. It is later redesigned into the Periodic system of elements (PSE) that shows atoms, ions, and even combined ions like nitrate or sulfate ions (see **Figure 1**). It now forms a part of the curricula of some German federal states and has also been internationally recommended within Senior-expert projects of teacher training abroad.

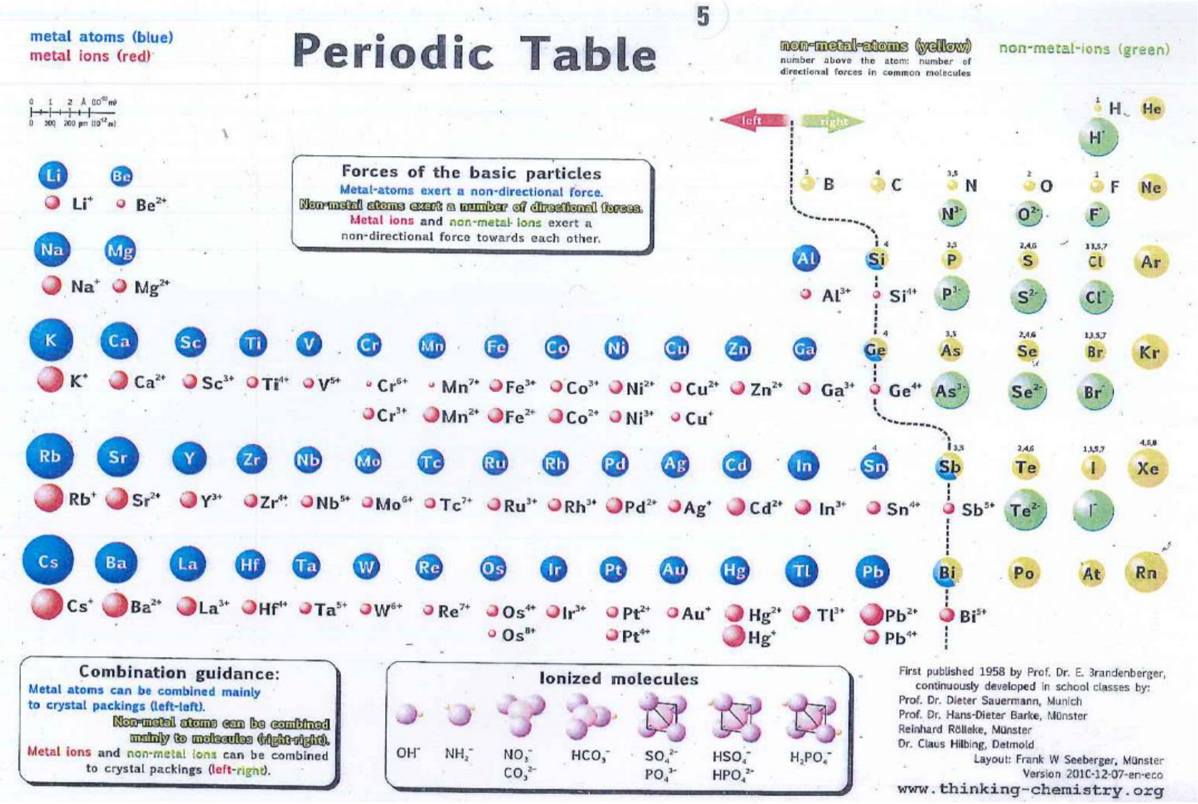


Figure 1. Didactical PSE of atoms and ions, combination rules, and combined ions.

By indicating the ions and their corresponding charge numbers, the PSE facilitates the students to determine formulas of salts on their own by simply taking electro-neutrality into account. In the case of the non-metal atoms, their respective quantities of bond forces are indicated (e.g. 4 for a C atom and 2 for an O atom). Regarding the N atom, two corresponding numbers are discussed: 3 for the N atom within an NH_3 molecule and 5 for the N atom within either an HNO_3 molecule or a nitrate ion. These numbers can be referred to as *standard bonding abilities*: They indicate the number of directional forces of non-metal atoms of one type that can be bonded by another atom.

The number 5 on the N atom (see **Figure 1**) has often been criticized because the indication of 5 bonds for the N atom is incompatible with the noble gas rule. That number 5 seems abnormal for anybody focused on electron pairs and the octet rule. The numbers 3 and 5, however, do *not* relate to electron pairs but to the number of *bonding forces* or *standard bonding capacities*. To successfully distinguish the main differences, historical facts regarding both ways of describing the homopolar (covalent) bond are summarized in the following paragraphs.

Chemistry is one of the important subjects in schools. Based on our previous reports (Barke, 1993; Barke & Engida, 2001; Barke 2012; Barke, 2015; Barke & Büchter, 2018), here, the purpose of this study was to explain chemical bonding for students from simple bond forces to electron pairs.

2. METHOD

This study analyzed the historical way from the first molecular models at the end of the 19th century based on *bond forces* between atoms in a molecule – no electrons or electron pairs are known by the scientific community. Later until the 1930s physicists and chemists developed the differentiated atomic model and introduced *electron pairs*: bonding and free electron pairs. Arrhenius created 1884 the ionic concept by measuring and comparing the electrical conductivity of salt solutions, and with Laue and Bragg in 1912 and 1914 it was evident that in solid salt crystals, the ions exist. This idea is not reaching all students today.

This long historical way was discussed with students of University Münster in the seminar: “Big steps in Chemistry history”. Each student took a famous Chemistry scientist like Lavoisier, Dalton, Kekulé, Liebig, or others, and presented their ideas for discussion.

3. RESULTS

3.1. Historical Model of Bonding Forces

Measuring "equivalent weights of elements in compounds" in the early 19th century led to the conclusion that an atom is always attached to a special number of other atoms. In 1860, and other scientists of his time introduced the term *valence*. They realized that the C atom is *tetravalent* concerning its attachment to H atoms, the “tetravalent C atom” binds either four H atoms to a CH_4 molecule or two O atoms to a CO_2 molecule.

Discovered the ability of carbon atoms to form chains and rings of C atoms, the “fruitful work in Organic chemistry” began. It is well-discussed by.Two-dimensional formulas were created and applied to the discussion of isomerism problems (**Figure 2a**), furthermore, the structure of the benzene molecule was proposed (**Figure 2b**).

Solved isomerism problems through the spatial tetrahedral concept of a methane molecule, he consequently proposed corresponding three-dimensional structural formulas and finally discovered the asymmetric C atom (**Figure 3**). "The findings about the *connecting forces* or *valences of atoms* became basic prerequisites for the elucidation of the structure of most important hydrocarbons".

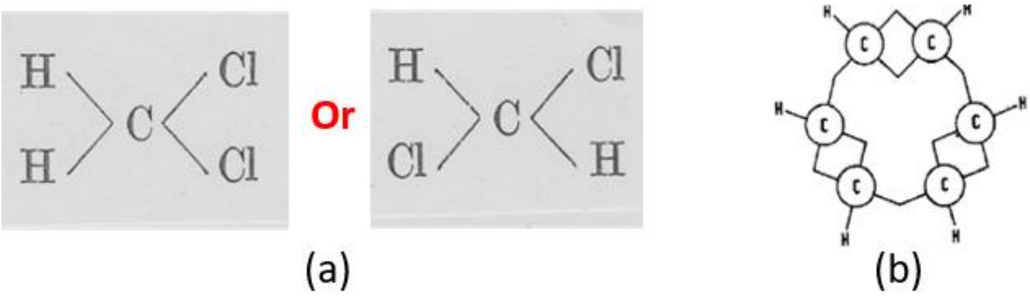


Figure 2. (a) Isomerism problems with CH_2Cl_2 molecules and (b) Kekulé's benzene structure. Figures (a) and (b) are adapted from Strube (1976) and Bugge (1955), respectively.

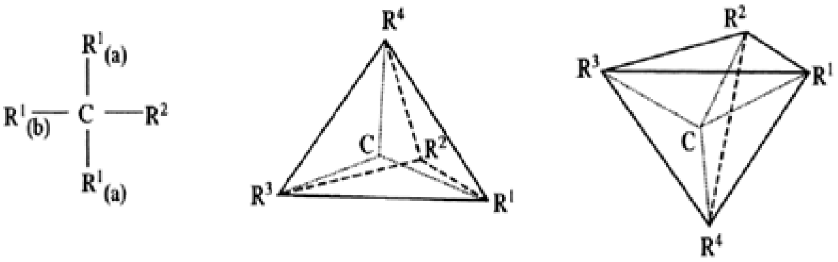


Figure 3. Tetrahedron model for mirror image isomerism.

All these basic ideas went without the electron concept which was not defined until the end of the 19th century, and by 1920 – 1930 firstly related and interpreted for chemical bonding. Yet, the 21st edition of the textbook of (later Holleman-Wiberg) exclusively mentions the valences of atoms instead of centering the now common electron term for chemical bonding. Therefore, just as still in 1955, structural formulas of important acid molecules were defined with valences; the N atom could thus quite well be "pentavalent" with 5 bond valences (**Figure 4**).

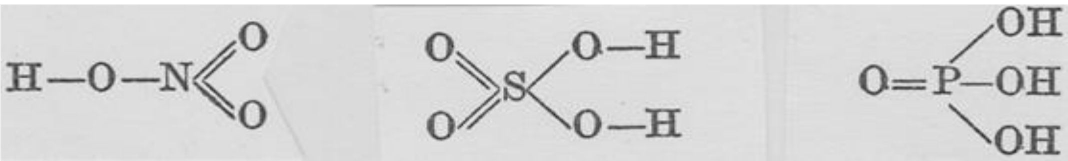
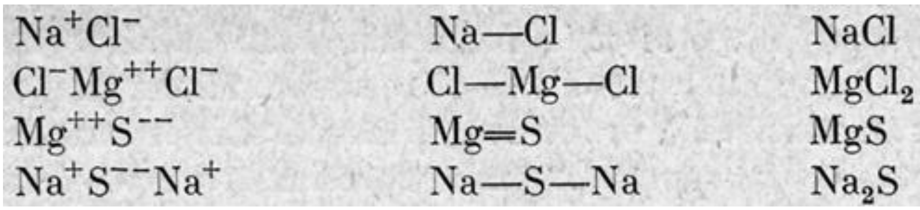


Figure 4. Molecular structures for acids.

In the foreword of the Holleman-Wiberg edition of 1943, it says: “In Inorganic chemistry, the valence line formulas have proven to be largely inadequate, and in numerous cases even false and misleading. Nevertheless, by far most of the inorganic textbooks still revert to this aid”. Assuming from their known tradition, many authors mingled new ion formulas with the misleadingly provided hyphens in molecule formulas (**Figure 5**). It was, however, clear since The molecular term does not apply to salts, because of their different constitution, namely ionic bonding in an ionic lattice.



Na^+Cl^-	$Na—Cl$	$NaCl$
$Cl^-Mg^{++}Cl^-$	$Cl—Mg—Cl$	$MgCl_2$
$Mg^{++}S^{--}$	$Mg{=}S$	MgS
$Na^+S^{--}Na^+$	$Na—S—Na$	Na_2S

Figure 5. Ionic symbols versus molecular formulas of solid salts until 1943.

It is well known that *physicists* (not chemists) have always followed the experimental aim to gain more and more insights into the interior of atoms. A successful model was developed by Bohr in 1913. The bottom line of this model was that the so-called electrons in the atom were assigned *different energies*, which are characterized by different spectra.

Since for physicists, "orbits" of the Bohr model symbolize *energy levels* of the electrons, it seemed logical to regard the "external, energy-richest" electrons for binding atoms in molecules and to expect a stable *energy minimum* for the entire electron system. This thought was the starting point for successful *energetic calculations* based on quantum mechanics. Nowadays, the calculation of bonds and molecules is standard among theoretical physicists and chemists. In the *simplest cases,* the energy minimum *in the calculation* symbolizes the four electron pairs. These were welcomed by chemists as the ordering principle for describing the homopolar bonding and designated as the "octet rule".

After introducing chemical bonding based on electron pairs, "Every shared electron pair, i.e. every atomic bond, is identified by a valence line starting from the atom in question. In many cases it is useful to reproduce free electron pairs using cross-directed lines" (**Figure 6**). This notation was later incorrectly extended to ionic salt compounds, such as chlorates, sulfates, phosphates, and silicates (**Figure 7**).

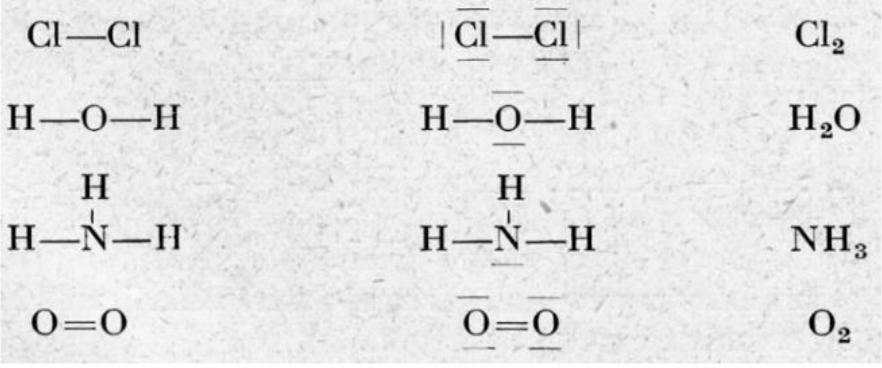


Figure 6. Valence lines for bond forces (left), for bonding and free electron.

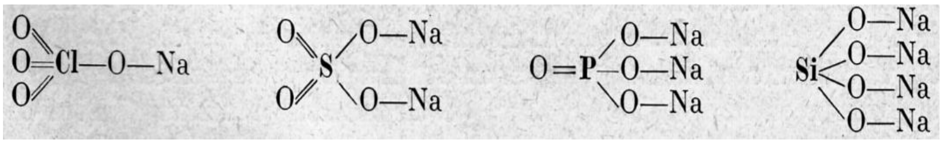


Figure 7. Valence lines and structural formulas of ionic lattices of salts.

Such "salt molecules" are corrected by newly introduced formulas for "*limiting structures*" with Mesomerism double arrow. This should express that the true structure exists between those others. The N-atom within nitrate ions and in nitric acid molecules is thought to be tetravalent so the octet rule and noble gas rule are fulfilled (**Figure 8**). To fulfill the octet rule, young learners are exposed to these complex limiting structures with the Mesomerism double arrow. Meanwhile, in addition to limiting structures, the edition of 1976 also strongly focuses on *bond numbers,* and with this, both concepts of chemical bonding are mixed (**Figure 9**). The correct way, however, is to assign bond numbers to valence formulas. For example, the bond number 1,5 indicates that all SO-bonds in sulfate ions are equal in length and that there are no single bonds located next to double bonds (**Figure 9**). The same applies to C-C-bonds in the benzene molecule.

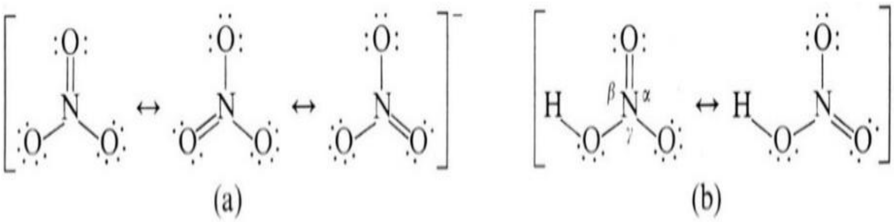


Figure 8. Limiting structures for nitrate ions and nitric acid molecules.

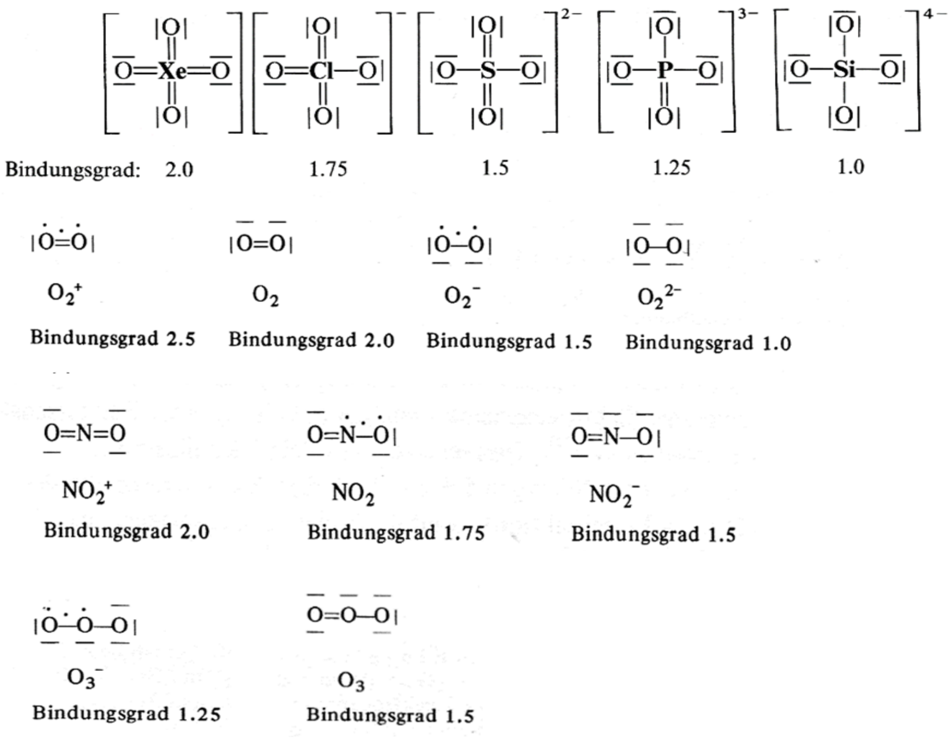


Figure 9. Limiting structures and bond numbers today.

The valence lines from the 19th century are tacitly used for electron pairs and thus provoke the confusion that there should not be an N atom with five valences. The didactical periodic table **(Figure 1)**, however, consistently refers to the model of standard bonding abilities – and correspondingly to 5-bond N atoms. Based on this, the next chapter explains how the didactical PSE of atoms and ions can be used.

3.2. The Bond Model of Valences for Teaching and Class

After introducing the properties and initial reactions of various substances, school curricula usually introduce Dalton's atomic model and the first atomic and molecular symbols: C and O, H_2 and O_2, H_2O and CO_2, etc. Since salts and salt solutions are also introduced at an early stage, it would be appropriate to use the ion term – nonetheless, it is argued that this is impossible before the introduction of the core-shell model of atoms.

With the didactical PSE (**Figure 1**) and the definition of the ion as an electrically charged particle with a certain ionic charge, it is possible to argue professionally about salt crystals and their ionic structure. Combinations of positively and negatively charged ions following the law of electro neutrality allow the derivation of salt formulas: Na^+Cl^-, $Ca^{2+}(Cl^-)_2$, $Al^{3+}(F^-)_3$ or $(Al^{3+})_2(O^{2-})_3$ as well as $NaCl$, $CaCl_2$, AlF_3 or Al_2O_3.

Analogically, non-metal atoms should be combined according to simple rules (with exceptions). For this purpose, *standard bonding abilities* are assigned. These are based on experimental data and depend on their group affiliation, for example, 4 for C atoms, 3 to 5 for N atoms, 2 to 6 for O atoms (or their homologs), and 1 to 7 for F atoms (or homologs). However, the bonding ability of 1 is known exclusively for H atoms and F atoms, while O atoms - with exceptions – have the bonding ability of 2.

Since the N atom now also establishes five standard bonding abilities e.g. the HNO_3 molecule, both numbers 3 and 5 are placed above the N atom symbol (**Figure 1**). Now learners can derive the molecular structures that are usual in class and describe many organic substances with formulas. In particular, 2-dimensional structures for acid molecules can be created, e.g. the HNO_3 molecule with 5 bonding abilities of the N atom (**Figure 10**), as well as the structure of the benzene molecule (**Figure 11**). For a deeper understanding, 3-dimensional models should be supplied through molecular model kits – see examples of sulfuric acid and nitric acid molecules (**Figure 12**), see also sphere packings of face-centered cubic structures like Cu-type and the NaCl-type). Apart from that, all those models should be discussed or even to be constructed by learners: they can build up their mental model in the cognitive structure.

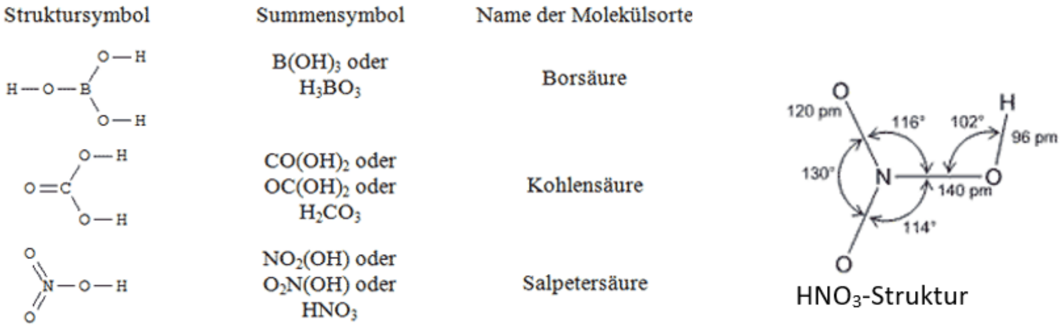


Figure 10. Structural symbols of some acid molecules.

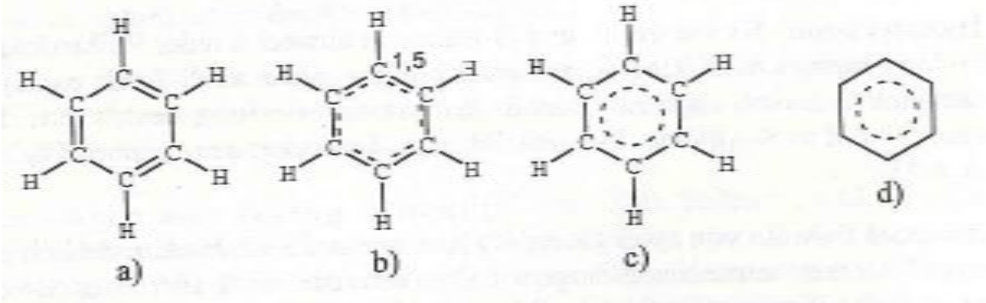


Figure 11. Structural symbols of the benzene molecule.

If learners are told using measurement results that bonding lengths in a molecule qualitatively represent the strength of the bonding between atoms, then rising force indicates rising standard bonding abilities. Between atoms of the same type, it can be noticed that the smaller the distance, the greater the force and thus, the greater the bonding strength.

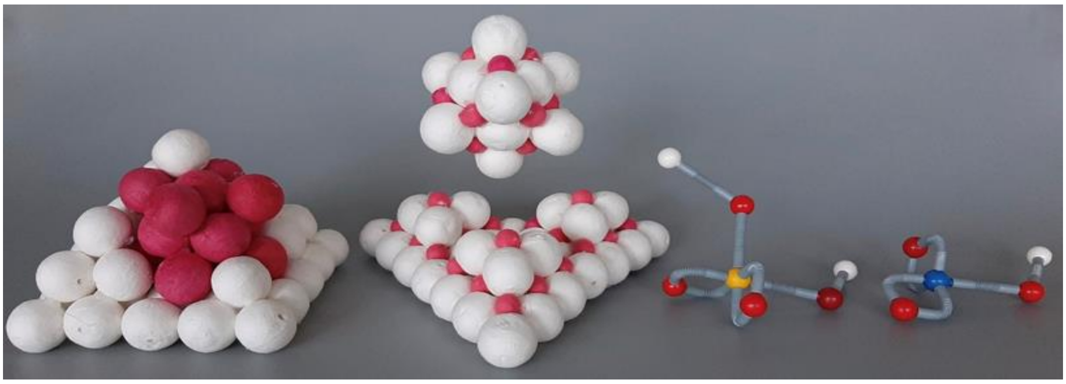


Figure 12. Sphere packing models for Cu and NaCl lattice, ball-and-stick models of H_2SO_4 - and HNO_3 molecules.

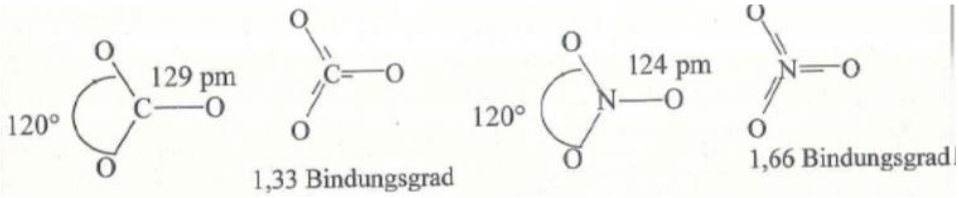


Figure 13. Chemical bonding through bond numbers in carbonate and nitrate ions.

Since all distances of C atoms within the benzene molecule are equal, the historic model of "oscillating single and double bonds" can be avoided and broken bond numbers should be chosen: The number 1.5 is represented by 1.5 standard bonding abilities between each of two C-atoms (**Figure 11)**. Carbonate or nitrate ions can also be correctly described with broken numbers of 1.33 and 1.66 (**Figure 13**).

The complexity of limiting structures in the electron pair model has already been visualized in **Figure 8**. In this respect, the model of standard bonding abilities is well-suited *for initial lessons* and can be successfully followed by learners. In the advanced instruction about the core-shell model of atoms and ions, the electron pair model can be usefully expanded by interpreting the valence lines in the simplest case as binding electron pairs and only free electron pairs should be explained additionally (Nandiyanto *et al.,* 2020; Nandiyanto *et al.,* 2021; Bilad & Prayogi, 2021; Wirzal & Putra 2022).

3.3. Implications for Chemistry Lessons

With these embodiments, there are three options regarding molecule structures that a teacher has to choose for their particular learning group:

(i) the exclusive introduction of binding abilities,
(ii) the introduction of both binding abilities *and* electron pairs,
(iii) the exclusive introduction of electron pairs.

In the first option, in this case, the didactical PSE of atoms and ions is introduced. With the help of metal atoms “left and left in the PSE”, metal and alloy structures can be developed easily. With the help of ion symbols “left and right in the PSE”, formulas of solid salts and corresponding ionic lattices can be deduced, and sphere packing models should be discussed. The PSE even provides the structure and charge numbers of some combined ions or “ionized ions” in hydroxides, nitrates, carbonates sulfates, and phosphates (**Figure 1**).

The numbers above the symbols of non-metal atoms are helpful for 2-D representations of many molecular structures, while 3-D models can be supplied through molecular model kits (**Figure 12**). For short training, for introductory courses of adult education, or chemistry class at school with only one hour per week, a basic comprehension of chemistry can be imparted – without extensive atomic models, its differentiated electron shells, and octet rule, and also without the complex electron theory of chemical bonding and limiting structures.

In the second option, after the introduction of bonding forces (see option 1), the core-shell model of the atom is introduced to reinterpret the already known binding lines as bonding electron pairs, while adding free electron pairs to the concept. Based on this, the octet rule is applied to the N-atom – such as for other non-metal-atoms – and complex limiting structures are implemented into the discussion (**Figures 8** and **9**).

Accordingly, the students have to deal with *two* models and discuss the question, of which of them is “the right one”: A comparison of both models as well as a discussion of similarities and differences of both concepts is mandatory, it should be clear that they are equivalent according to understand molecular structures – those models are not “right or wrong”. In doing so, however, learners can study the development of knowledge in science and understand the extension of models for the structure of matter: Starting from the tiniest particles like atoms, ions, or molecules up to the core-shell model and, if necessary, to the electron cloud model or atomic and molecular orbitals.

In the third option, if the bonding model of electron pairs is the only model to be taught, then chemical bonding can only be reflected quite late in the lessons of grades 10 or 11 after having developed enough knowledge of the differentiated atomic model. Until then, the usual formulas are written and learned more or less by heart without knowing the structures of the ionic lattices and molecules: Misconceptions about possible arrangements of atoms in molecules can arise, for example, "HHSOOOO" for the H_2SO_4 molecule (Barke & Büchter, 2018). Not to mention the structure of salts such as NaCl or $CaCl_2$: Ideas of “Na-Cl-molecules” or “Ca atoms and Cl_2-molecules in calcium chloride” have been empirically proven. Lessons according to option 3 should therefore work with many spatial structural models such as 3-D ionic lattices and 3-D molecular models (**Figure 12**) to overcome such misconceptions and to build up a scientific mental model in the cognitive structure of young.

In all cases, standard bonding abilities and electron pairs have to be regarded as two equivalent models for the description of chemical bonding and they should be discussed with learners. None of the models is right or wrong. If learners want to provide qualitative information, learners should choose standard bonding abilities. If learners want to calculate the energies of chemical bonding, learners must choose electron pairs.

4. CONCLUSION

Chemical bonding between the atoms of a molecule can be described in two independent ways that are comparable in chemistry: Bond forces and electron pairs. Standard bonding forces can be established in early chemistry in classes, such as four bonds in the case of the C atom within a CH_4 molecule or two bonds in the instance of the O atom inside an H_2O molecule. This is possible without having connections to the nucleus-shell model of atoms. Additionally, the ion concept can be reflected early in class if we use the special Periodic table with atoms and ions as basic particles of structure of matter. As a result, ideas for teaching chemistry are examined, and various methods of learning are contrasted.

5. AUTHORS’ NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. The authors confirmed that the paper was free of plagiarism.

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