BOND FORCES VERSUS ELECTRON PAIRS – TWO CONCEPTS FOR CHEMICAL BONDING

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ABSTRACT

In chemistry there are two equivalent ways of describing chemical bonding between atoms in a molecule: On the one hand there are *bond forces* and on the other hand there are *electron pairs*. In order to introduce chemical bonding already in early chemistry class without having to relate to the nucleus-shell model of atoms, *standard bonding abilities* can be defined – e.g. four bonds in case of the C atom within a CH_4 molecule or two bonds in case of the O atom within a H_2O molecule. Accordingly, proposals for Chemistry education are discussed and ways of instruction compared. *[African Journal of Chemical Education—AJCE 11(1), January 2021]*

INTRODUCTION

In the 1990s, our working group [1] developed and later redesigned [2] a special didactical periodic system of elements (PSE) which shows atoms and ions **(see Fig. 9 in this paper).** It now forms a part of curricula of some of the German federal states [3] and has also been internationally recommended within Senior-expert projects and teacher trainings abroad.

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 [1]. In 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 a NH_3 molecule and 5 for the N atom within either a HNO_3 molecule or a nitrate ion. These numbers can be referred to *standard bonding abilities*: They indicate the quantity of directional forces of non-metal atoms of one type that can be bonded by another atom [1].

The number 5 on the N atom **(see Fig. 9)** has often been criticized because the "indication of 5 bonds for the N atom is incompatible with the noble gas rule" [4]. That number 5 actually 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 quantity of *bonding forces* or *standard bonding capacities* [1]. In order to successfully distinguish the main differences, historical facts regarding both ways of describing the homopolar (covalent) bond are being summarized within the following paragraph.

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, **Kekulé** [5] and other scientists of his time introduced the term *valence*: They realized that the C atom is *tetravalent* in relation to 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.

When **Kekulé** discovered the ability of carbon atoms to form chains and rings of C atoms, the “fruitful work in Organic chemistry” began [6]: Two-dimensional formulas were created and applied on the discussion of isomerism problems (**Fig. 1a**). Furthermore, a variety of structures of the benzene molecule [5] were proposed (**Fig. 1b).**

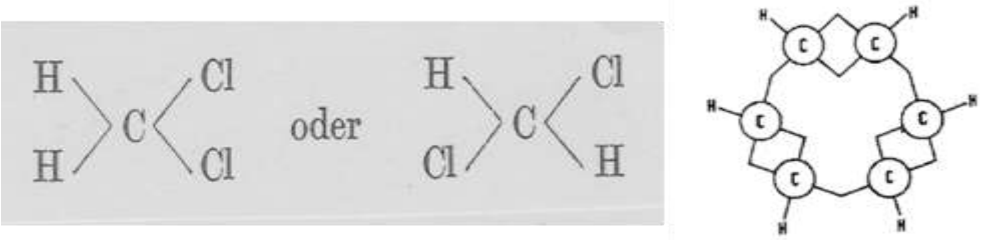


Fig. 1: a) Isomerism problems with CH_2Cl_2 molecules [6], **b)** Kekulé's benzene structure [7]

Van t'Hoff [8] 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 (**Fig. 2**). "The findings about the *connecting forces* or *valences of atoms* became basic prerequisites for the elucidation of the structure of most important hydrocarbons" [6].

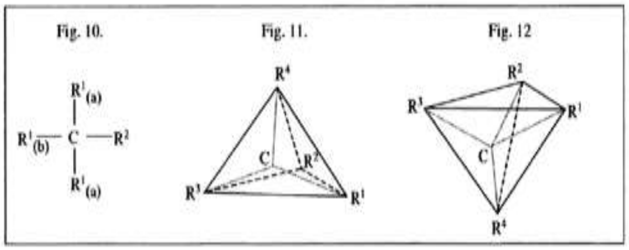


Fig. 2: Tetrahedron model for mirror image isomerism according to Van t'Hoff [8]

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 closer defined to chemical bonding. Yet, the 21st edition of the textbook of **Holleman** (later Holleman-Wiberg) from 1937 [9] exclusively mentions the valences of the atoms instead of centring the now common electron term for chemical bonding. Therefore – just as still in 1955 by **Remy** [10] – structural formulas of important acid molecules were defined with valences; the N atom could thus quite well be "pentavalent" with 5 bond valences (**Fig. 3**).

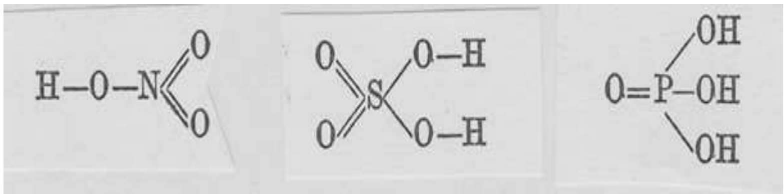
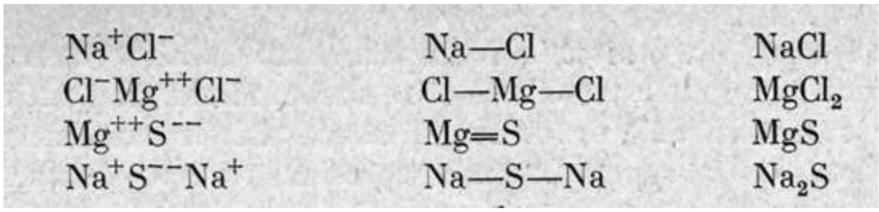


Fig. 3: Molecular structures for acids in textbooks until 1955 [10]

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” [11]. Assuming from their known tradition, many authors mingled formerly new ion formulas with the misleadingly provided hyphens in molecule formulas (**Fig. 4**). It was, however, clear since **Laue** and **Bragg** (1912) that the molecular term is not applicable 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

Fig. 4: Ionic symbols versus molecular formulas of solid salts until 1943 [11]

It is well known that the *physicists* (not the chemists!) have always followed the experimental aim to gain more and more insights of 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 where assigned with *different energies*, which are characterised 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 on the basis of electron pairs, **Holleman** and **Wiberg** state [11]: "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 by means of cross-directed lines" (**Fig. 5**). This notation was later incorrectly extended to ionic salt compounds, such as chlorates, sulfates, phosphates and silicates (**Fig. 6**).

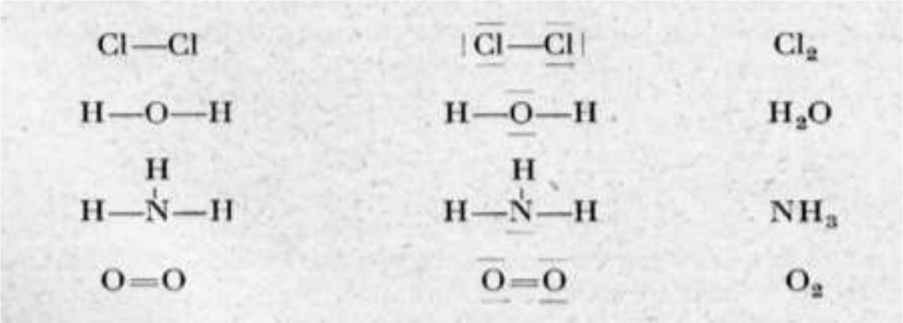


Fig. 5: Valence lines for bond forces, bonding and free electron pairs in molecules [11]

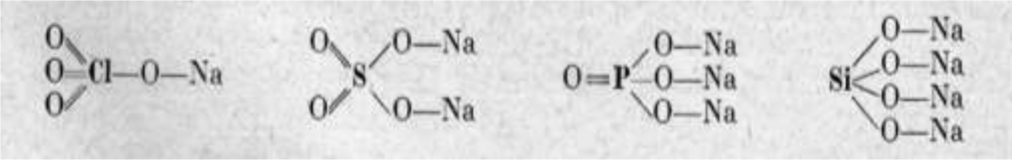


Fig. 6: Valence lines also for structural formulas of ionic lattices of salts [11]

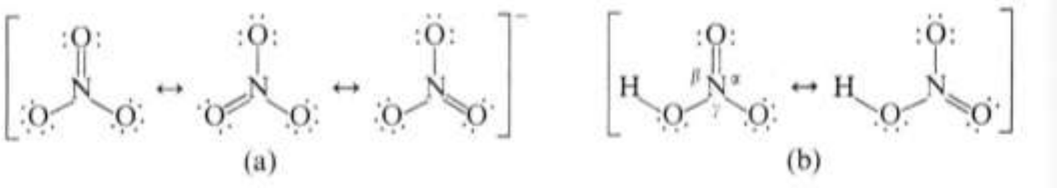


Fig. 7: Limiting structures for nitrate ions and nitric acid molecules [11]

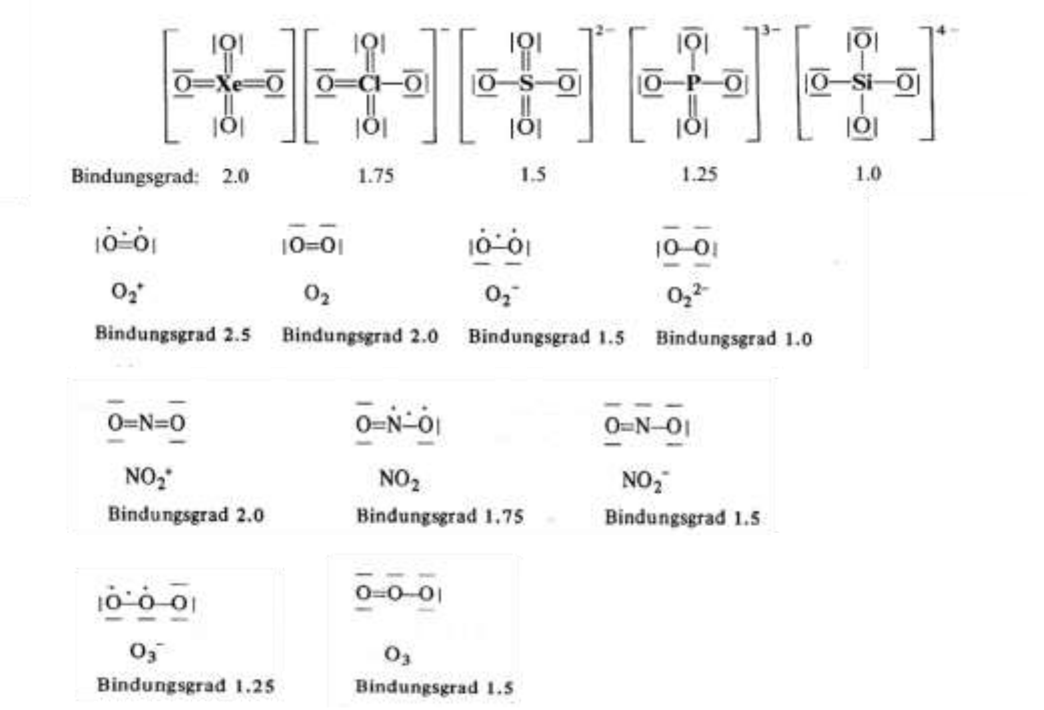


Fig. 8: Limiting structures and bond numbers [11]

In Holleman-Wiberg editions of 1943 to 2017, such "salt molecules" are corrected by newly introduced formulas for “*limiting structures*” with Mesomerism double arrow [11] – 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 that octet rule and noble gas rule are fulfilled (**Fig. 7**). In order to fulfil the octet rule, young learners are exposed to these complex limiting structures.

Meanwhile, in addition to limiting structures, the edition of 1976 also strongly focusses on *bond numbers* and with this, both concepts of chemical bonding are mixed with each other (**Fig. 8**). 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 sulphate ions are equal in length and that there are no single bonds located next to double bonds (**Fig. 8)**. The same applies to C-C-bonds in the benzene molecule.

It can be seen that 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 **(Fig. 9)**, however, consistently refers to the model of standard bonding abilities – and correspondingly the 5-bond N atom. Based on this, the next chapter explains the manner in which the didactical PSE of atoms and ions can be used [1].

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 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 (**Fig. 9**) 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 in accordance with the law of electro neutrality allows 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 [12].

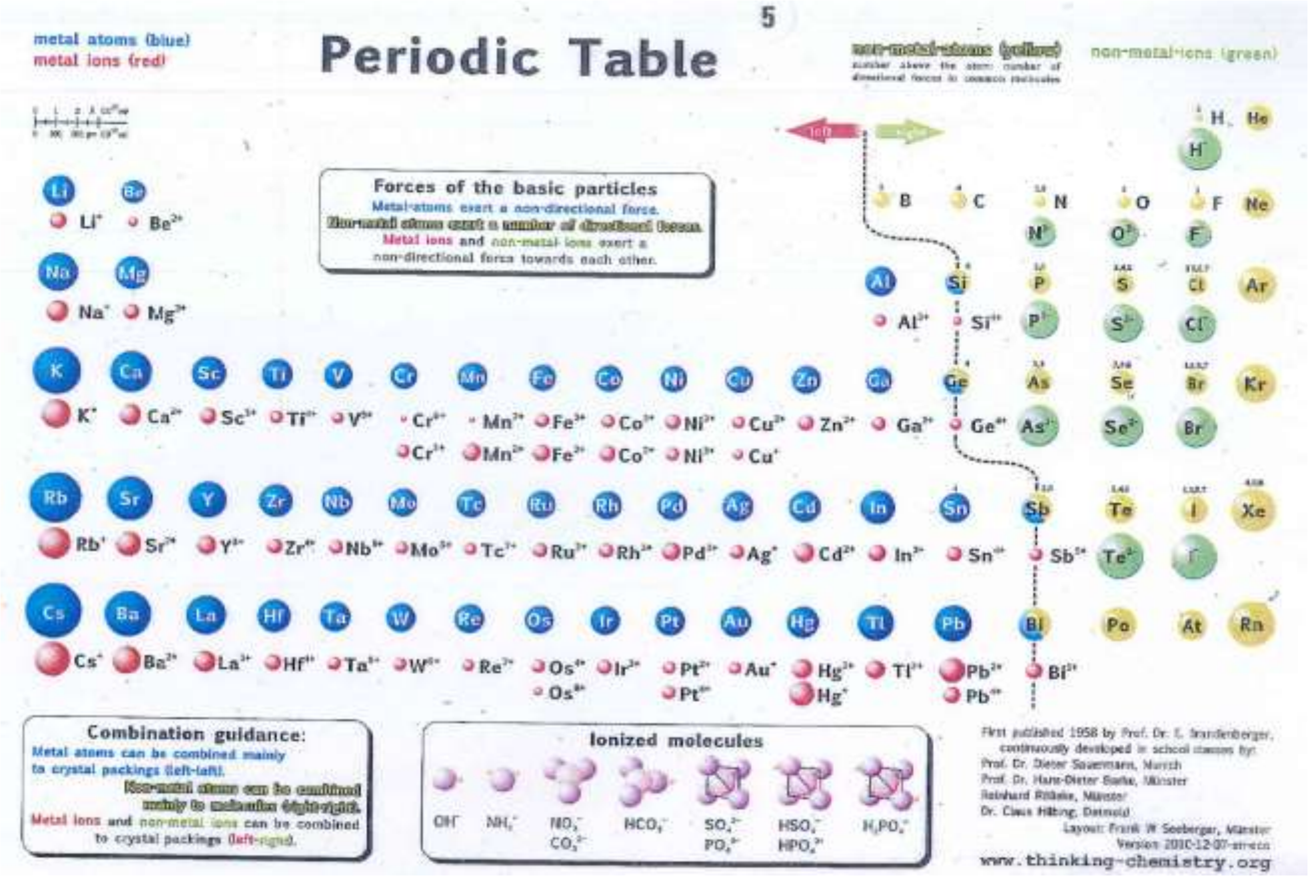
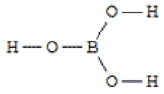
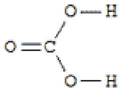
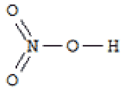


Fig. 9: Didactical PSE of atoms and ions, combination rules and combined ions [2]

Analogically, non-metal atoms should be combined with each other according to simple rules (with exceptions). For this purpose, *standard bonding abilities* are assigned to them. 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 their homologues). 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 for e.g. the HNO_3 molecule, both numbers 3 and 5 are placed above the N symbol **(Fig. 9)**. Now learners can derive the molecular structures that are usual in class and describe many organic substances with formulas [12]. 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 (**Fig. 10),** as well as the structure of the benzene molecule (**Fig. 11**). For deeper understanding, 3-dimensional models should be supplied through molecular model kits – see examples of sulfuric acid and nitric acid molecules (**Fig. 12**, see also sphere packings of face-centred 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 [12].

Struktursymbol	Summensymbol	Name der Molekülsorte
	$B(OH)_3$ oder H_3BO_3	Borsäure
	$CO(OH)_2$ oder $OC(OH)_2$ oder H_2CO_3	Kohlensäure
	$NO_2(OH)$ oder $O_2N(OH)$ oder HNO_3	Salpetersäure

HNO_3-Struktur

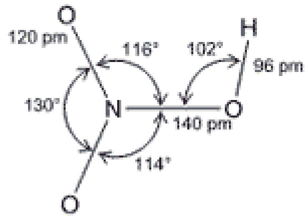


Fig. 10: Structural symbols of some acid molecules [1]

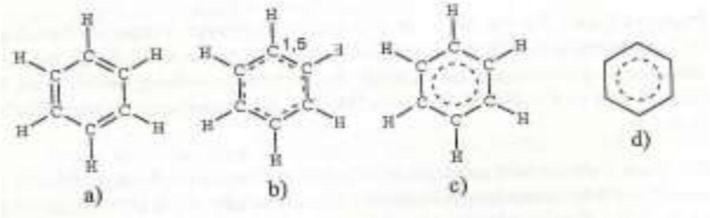


Fig. 11: Structural symbols of the benzene molecule [1]

If learners are told by means of 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: The smaller the distance, the greater the force and thus, the greater the bonding strength.

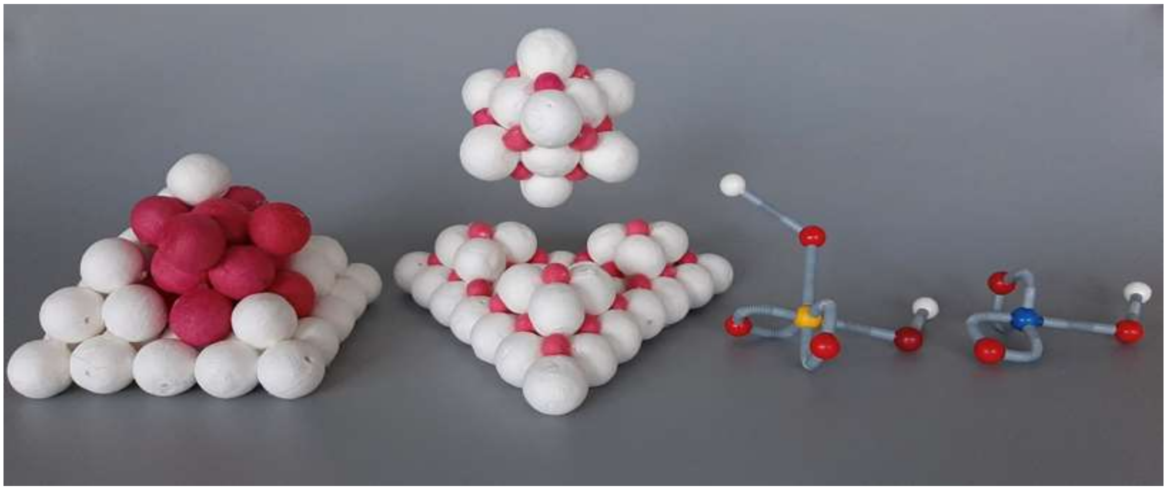


Fig. 12: Sphere packing models for Cu and NaCl lattice, ball-and-stick models of H_2SO_4 - and HNO_3 molecules [13]

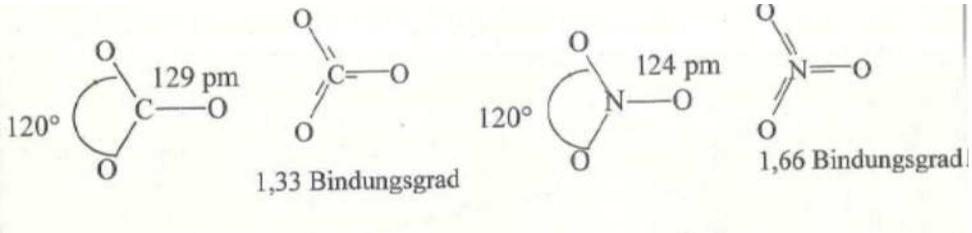


Fig. 13: Chemical bonding through bond numbers in carbonate and nitrate ions [1]

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 two C-atoms (**Fig. 11 b)**. Carbonate or nitrate ions can also be correctly described with broken numbers of 1.33 and 1.66 (**Fig. 13**).

The complexity of limiting structures in the electron pair model has already been visualized in **Fig. 7**. 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.

IMPLICATIONS FOR CHEMISTRY LESSONS

With these embodiments, there are three options regarding molecule structures which a teacher has to choose for their particular learning group: 1) the exclusive introduction of binding abilities, 2) the introduction of both binding abilities *and* electron pairs or 3) the exclusive introduction of electron pairs.

Option 1) 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 [1] can be developed easily. With the help of ion symbols "left and right in the PSE", formulas of solid salts and corresponding ionic lattices [1] can be deduced, 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, sulphates and phosphates **(Fig. 9)**.

The numbers above the symbols of non-metal atoms are helpful for 2-dimensional representations of many molecular structures, while 3-dimensional models can be supplied through molecular model kits **(Fig 12)**.

For short trainings, for introductory courses of adult education or for chemistry class at school with only one hour a 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.

Option 2) After introduction of bonding forces (see option 1), the core-shell model of the atom is introduced with the aim of reinterpreting 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 discussion (**Fig. 7** and **8**).

Accordingly, the students have to deal with *two* models and discuss the question, which of them is "the right one": A comparison of the models as well as a discussion of similarities and differences of both concepts is mandatory. 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 tiniest particles like atoms, ions or molecules up to the core-shell model and, if necessary, the electron cloud model and to atomic and molecular orbitals.

Option 3) 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 ion lattices and molecules: Misconceptions about possible arrangements of atoms in molecules can arise, for example "HHSOOOO" for the H_2SO_4 molecule. 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 [15]. Lessons according to option 3 should therefore work with many spatial structural models such as 3D ionic lattices and 3D molecular models to overcome such misconceptions and to build up a scientific mental model in the cognitive structure of young learners [16].

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 you want to provide qualitative information, you should choose standard bonding abilities; if you want to calculate energies of chemical bonding, you must choose electron pairs!

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