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Chemistry: A Bunch of Symbols?

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Abstract: Teaching and learning chemical formulas and structures is challenging. In many cases students understand chemical formulas only at a superficial level and poorly comprehend and retain the underlying chemical processes. Teaching methods still follow historically evolved principles, which are briefly summarized in this article. Difficulties and misconceptions that students encounter are presented and discussed. Didactic principles are proposed to help overcome the main challenge of connecting learned concepts and models to chemical formulas. The macOS and iPadOS application MoleculeSketch for drawing chemical structures is presented.

Keywords: Chemical education · Chemical formulas · MoleculeSketch

Stefan Dolder studied Chemistry at the University of Bern. In his master thesis and PhD he investigated tetrathiafulvane (TTF) based ligands and their transition metal complexes as multifunctional materials with conducting, magnetic and optical properties under the supervision of Prof. Silvio Decurtins. During his PhD he also obtained his diploma for teaching at higher secondary schools for chemistry (*Höheres Lehramt*). Since 2006 he teaches chemistry at the *Gymnasium und FMS Lerbermatt*. As a side project he developed the macOS and iPadOS application MoleculeSketch for drawing chemical structures, for which he was awarded the Balmer Prize of the Swiss Chemical Society for innovations in the teaching of chemistry in 2023.

1. Introduction

During a school trip to Genoa a fresco on the ceiling of a former pharmacist's apartment struck my attention. An angel is holding a book with strange symbols (Fig. 1).

The depicted glass flask and the title page of '*Elementary Treaties on Chemistry'* by Lavoisier in the right corner made it clear that those must be alchemical symbols. But what do they mean?

Although modern chemical symbols offer a more familiar description of chemical compounds and reactions with the use of letters from the Latin alphabet instead of cryptic characters, they are nonetheless still challenging to understand. Chemists easily forget how much about their language is not obvious, just as native speakers of any language are unaware of the linguistic rules applied automatically.[1a]

It is an important task as chemistry teacher to introduce students to the symbolic chemical language. Chemical symbols, formulas and equations allow us to write down the essence of observations from experiments and to discuss and understand the chemical processes that lead to these observations. Teachers must help students connect the symbolic language of chemistry with the macroscopic world of experience and the microscopic world in which much chemical thought takes place.[1b] If this fails, students are forced to process chemical language at a superficial level and to focus on the symbols rather than the ideas the symbols convey. The material is poorly understood, poorly retained, and frequently confused.[1c]

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Fig. 1. Fresco on the ceiling of a former pharmacist's apartment in Genoa. In the center of the picture an open book held by an angel with alchemical symbols is visible. In the bottom-right corner, a second book with the inscription '*Lavoisier Trattato Elemente di Chimica*' is shown. The inscription on the top is a quote from Horace (Carmen III, 24, 31-32): *virtutem [incolumem odimus], sublatam ex ociulis quaerimus invidi (engl.:* [We hate] virtue [when it is safe], when removed from our sight we long for it jealously). Photo credit: S. Dolder.

2. Historical Evolution of the Symbolic Chemical Language

Up to the 18th century alchemical symbols were used to describe chemical compounds and reactions. Only insiders knew their meaning and while some commonly used symbols existed, like for the four elements water, fire, earth, and air or for compounds like sulfur, phosphorus, or acetic acid, many different symbols were sometimes used for the same compound to keep the knowledge secret (Fig. 2). These symbols were merely labels, completely arbitrary and did not provide information about the composition or structure of the compounds.[2]

By linking the concepts of elements and atoms together, Dalton developed circular elemental symbols that allowed him to formulate chemical reactions as combinations of these symbols in his 1808 treatise '*A New System of Chemical Philosophy'*. With his assumption of spherical atoms, he paved the way to better understand the atomic composition of compounds. Nevertheless,

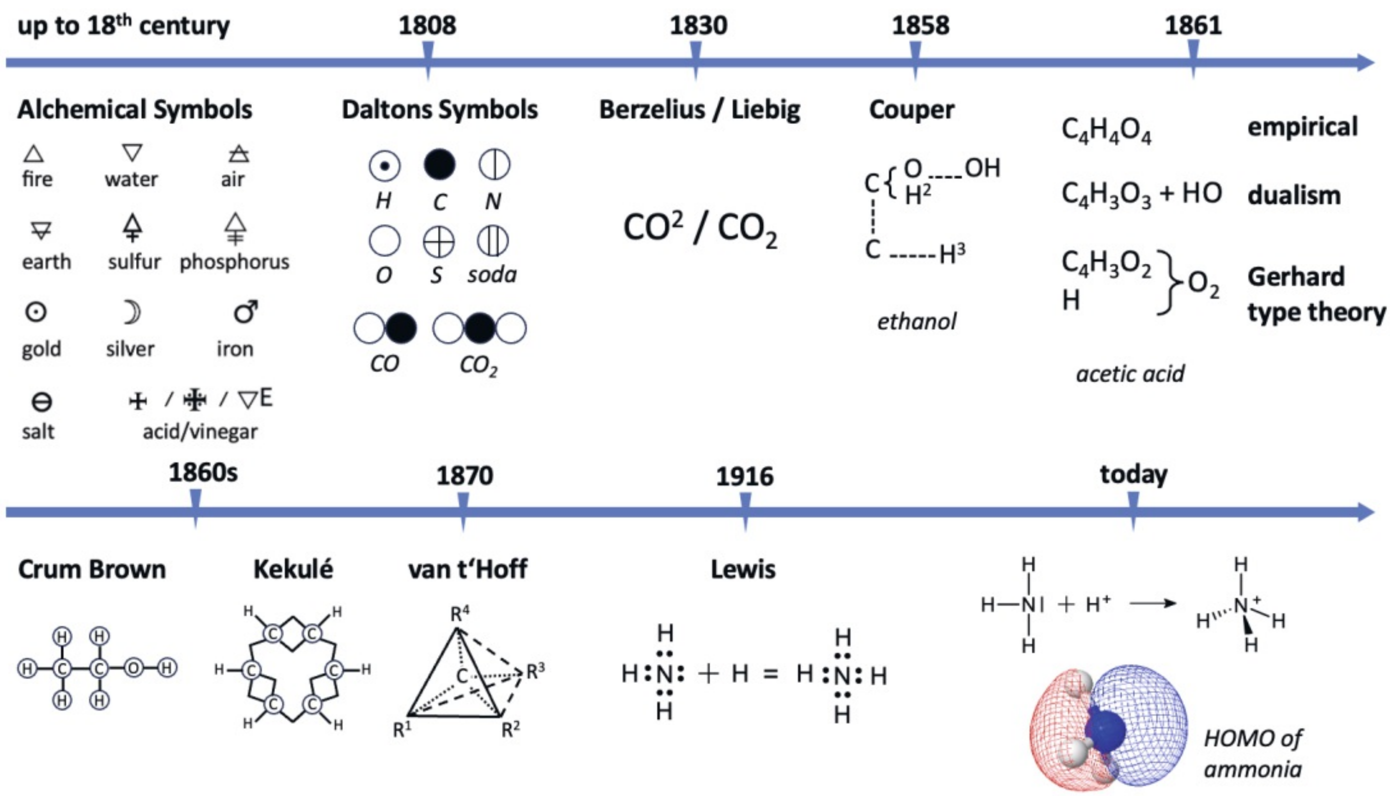

Fig. 2. Overview of the historical evolution of chemical symbols, formulas and structures (3D structure and HOMO calculated using MolCalc).[2,6,7]

Dalton's symbols were still cumbersome to use, and it was Berzelius who proposed to use ordinary letters linked to the Latin name of the elements in 1813, making them easy to remember and write.[3] Following the work of Avogadro and Cannizzaro a further step in the systematization of chemical formulas was taken at the congress in Karlsruhe in 1860, which led to the modern distinction between atoms and molecules. Formulas used by that time were primarily empirical and described the mass ratio between the present elements.[2] While Berzelius used numbers in superscript to express these mass ratios, it was Liebig in the 1830s who introduced subscripts in empirical formulas as they are still used today.

Advances in chemical analysis brought isomers and functional groups, then called radicals, to the chemical community's attention, which could not be described with empirical formulas. Several theories like dualism, type and radical theory were produced in the attempt to explain these phenomena, leading to many different forms of chemical representations once again. In 1852 Frankland proposed the concept of valence to explain why elemental substances always react in the same mass ratios. Kekulé's insights in 1857 to expand the concept of valence to the way atoms bind to each other, and the introduction of the tetrahedral model in 1867 for the carbon atom were the basis for the structural perception of chemical formulas. With the work of Couper, who proposed drawing lines between the letters to symbolize bonds, as well as Crum Brown, Butlerow, Van t'Hoff and LeBel, the notion of structural formula, as we use them today, was born in the late 1870s.[4]

Although the chemical bond may have been a mere abstraction in the mind of chemists at that time and the nature of the chemical bond remained mysterious, the hypothesis of the bond was however amply justified by the signal adequacy of the simple theory of molecular structure to which it gave rise.[5] With the discovery of subatomic particles and the atomic structure it became clear that electrons must be involved in the formation of the chemical bond. This was rationalized in 1916 with Lewis' theory of electron pairs which led to the famous Lewis structures.[6] Whereas Lewis mainly used pairs of dots to symbolize all electron pairs, lines to represent bonds prevailed over time and only free electron pairs are drawn as dots today. Although in several language areas, like German or French, free electron pairs are drawn as lines too. The need to illustrate the more and more complex molecular structures brought to light by modern measuring or theoretical methods, like X-ray crystallography, led in the middle of the 20th century to the development of enhanced and mixed forms, like the skeletal formula, Natta or Fisher projections. As computers and quantum mechanical computations began to be broadly available in recent times, 3D structures, molecular orbital structures, and computer-readable chemical notations, like SMILES or InChI line notations, are nowadays widely used to illustrate and investigate chemical structures.

3. Challenges in Teaching Chemical Formulas and Common Student Misconceptions

But where to start teaching chemical formulas to students? In the German-speaking parts of the world, textbooks and chemistry curricula usually start with states of matter and their properties. Properties are rationalized by introducing and applying particle theory. Chemical reactions are used to explain the notion of elements and compounds and simple chemical reactions are formulated. Up to this point, in most cases chemical symbols and formulas have not been used. The substances in the chemical equations are written as words. It is only after introducing Dalton's atomic theory that the first chemical symbols in form of labels for elements are shown. From the notion that atoms are rearranging during a chemical reaction, compound formulas are used to write down stoichiometrically equilibrated chemical equations. Usually, students struggle at this point not only to find out the correct coefficients but more generally to understand the meaning of the symbols they have to read or write. For many it seems as if they have to deal with almost arbitrary letters and numbers, some capitalized some not, some numbers positioned as subscripts, some written before the letters.

As teaching experience shows, common mistakes are misspelling or misinterpretations of element symbol, like Co instead of CO or, depending on the font used, C + I_2 in Cl_2 instead of two chlorine atoms. Instead of adapting the coefficients, the numbers in the chemical formulas are often altered to satisfy the equation or the numbers are assigned to the wrong element (Fig. 3).

These problems may have various causes. Chemical terms, and therefore chemical formulas, are strongly tied with chemical concepts and models. Teaching will be effective so long as the students are already familiar with the concepts to which the terms belong or can connect the terms to the concepts.[1d] When trying to understand chemical reactions, students must deal with many concepts. On one hand, the symbols stand for elements or atoms. Elements may be understood as substances or types of atoms. On the other hand, compound formulas may be interpreted as some kind of abbreviation for a chemical substance instead of the name of the compound, or as an indication of the atomic composition. Many conventions need to be considered, like the order of letters and numbers. Added phase symbols or information about energy conversion, mathematical and Greek symbols must be understood. All these considerations make deciphering chemical symbols difficult and should be addressed by the teacher.

Most of the time students already know some chemical formulas from their prior education or everyday life experience. The formulas are already tied to some concept in their mind. From a constructivist approach those preconceptions need to be considered to allow students to successfully learn the new meaning of chemical formulas by altering or enhancing their previous knowledge. Therefore, it is crucial that teaching and exercising should not only focus on the technical aspects, like finding out the right stoichiometric coefficients in an equation, but also explain and ask for the purpose and meaning of chemical formulas.

The purpose of chemical formulas at this stage is to describe chemical change on a macroscopic and atomic level and to enable students to do stoichiometric mass calculation to predict substance amount in chemical reactions. To understand the nature of the forces holding the atoms together, the structure of an atom, subatomic particles and Coulomb's law on electrostatic force must be learned. The elemental symbols in chemical formulas may now be describing ions of a salt, or the formula represents a molecule that can be written as a Lewis structure. The amount of information that can be deduced from a chemical formula increases even more. Lewis structures add more symbols to be deciphered, like lines, charge, or partial charge indicators. Lines in Lewis structures have different meanings. They may be bonds, free electron pairs or even part of chemical symbols as letters L or I.

Common mistakes like writing Lewis structures for salts or ignoring the valence of atoms when drawing molecular bonds are clues that the bonding models have not been fully understood (Fig. 3). Further confusion may arise when different chemical representations are confused, like parts of condensed formulas in Lewis or skeletal structures as abbreviation of functional groups.

Even more challenges emerge when studying the 3D structure of chemical compounds. To understand the spatial arrangement of atoms in molecules or even biomolecules notions of the VSEPR model, stereoisomerism, hydrogen bonds and new forms of depiction like ball and stick models or ribbon diagrams must be understood.

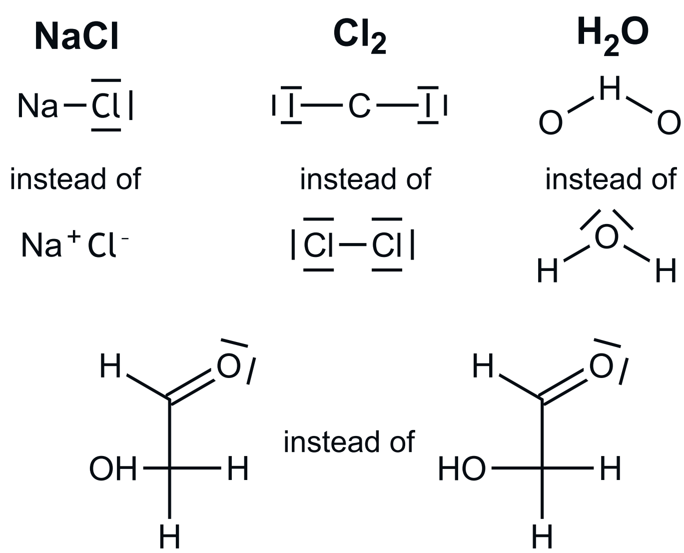

Fig. 3. Common mistakes made by students.

4. Developing a macOS and iPadOS App to Draw 2D Chemical Structures

When preparing a chemistry lesson, scripts, slides, or exercises for appropriate chemical formulas are needed. All too often formulas found on Wikipedia or the internet in general are not exactly drawn in the way the teacher wants. Online, browser-based 2D chemical drawing applications like ChemDraw JS,[8] ChemDoodle[9] or Marvin JS[10] offer limited or inadequate features. On Apple platforms common free or commercial applications are not easily available.

If there is no suitable program, why not develop one myself? Following this simple idea, the development of MoleculeSketch[11] began (Fig. 4). Alongside programming skills in Objective-C and later on Swift and SwiftUI, I quickly realized that developing a drawing program involves much more than writing program routines. A file format had to be created to be able to save the drawings locally and later also in iCloud. Designing an easy-to-use graphical interface, writing help pages and a homepage, translating the program into English and French, distributing the program *via* the App Store, and providing customer support for questions and problems were challenges to be met.

In contrast to many other programs, free electron pairs, oxidation numbers and partial charges can be displayed automatically. It is possible to calculate the average molecular mass and formula automatically. Abbreviations for commonly used functional groups can be expanded into structural formulas. Chemical drawings may be copied or exported into other applications as images or PDF files. There is even the option to import structure files from external sources such as MOL or SDF files.

Although standard commercial chemical drawing programs may offer more functionality, connection to databases, and import and export possibilities, user response shows that MoleculeSketch with its core functionalities meets most of the needs for scientific writing while being easy to use.

MoleculeSketch is not a collaborative environment. It is designed to be used by a single user on Apple platforms. For educational or teaching activities a browser-based learning environment like Zisimos may be better suited.[12]

5. Final Remarks and Didactic Suggestions

It is easily forgotten that chemical structures and formulas are not self-explanatory for students and require a sophisticated understanding of complex chemical models, concepts and rules. Following experiential principles these are my suggestions to assist students in becoming more proficient and confident while using chemical symbols and formulas:

- State clearly what purpose and meaning chemical symbols, formulas or equations have in the applied context.
- Clearly differentiate between macro- and microscopic level and terms like element, atom, ion, finite (molecules) and infinite (lattices) structures.

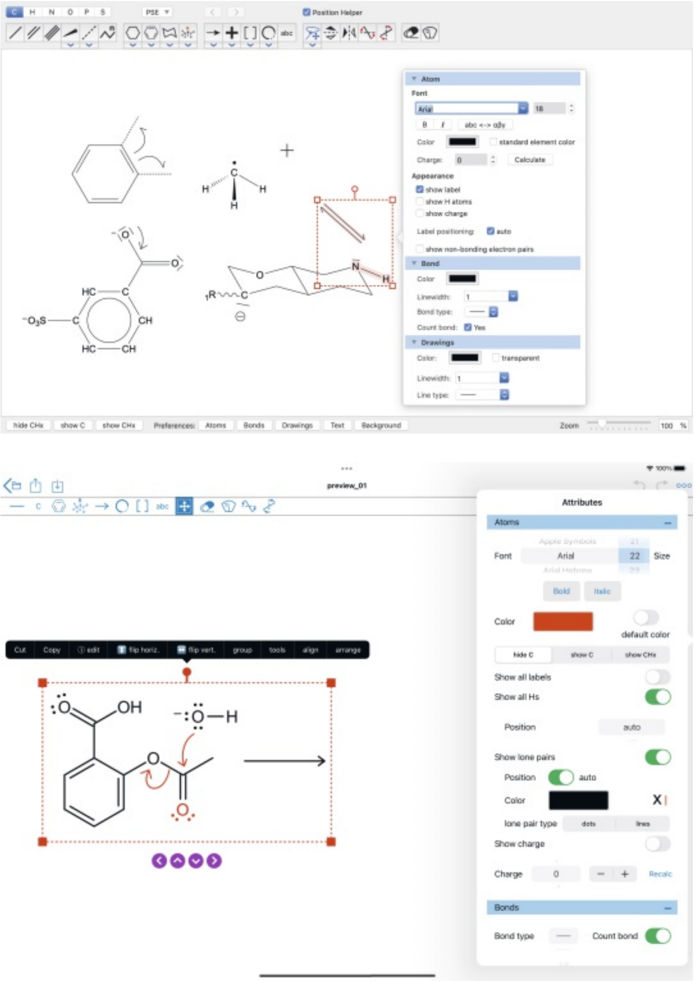

Fig. 4. Screenshots of MoleculeSketch for macOS (top) and iPadOS (bottom).

– Use comprehension and not only technical or procedural questions in exercises.
– Avoid mixed or incomplete forms of illustration and use consistent and appropriately drawn chemical formulas or structures.
– Use scaffolding methods to provide helpful hints or definitions of special symbols, or scientific vocabulary.
– Apply visual or tactile models to let the students experience the concepts and spatial structure conveyed by chemical formulas.

This should help to form the connection between the symbols and the previously learned ideas and concepts, and hence facilitate processing chemical structures at a deeper level of understanding.

Teaching environments on electronic devices that provide an adequate, easy to use, and accessible way to learn chemical formulas and structures are not available yet. Recent advances in AI and AR technologies like chatGPT or different VR/AR headsets may provide new opportunities.

6. What Do the Alchemical Symbols in the Fresco Mean?

Finally, one question remains unanswered: what do the alchemical symbols on the fresco mentioned at the beginning of this article mean? The following figure (Fig. 5) shows an attempt to decipher them. More insights or corrections are welcome and may be addressed to the author.

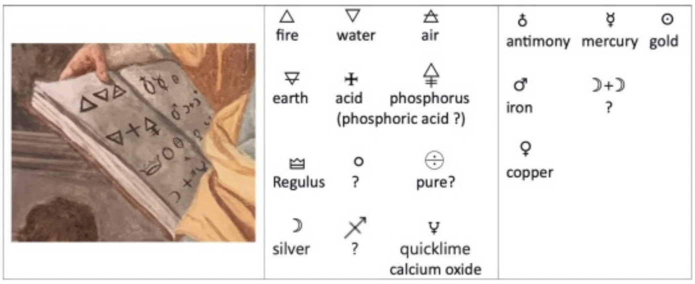

Fig. 5. Detail from the fresco in Fig. 1 with deciphered alchemical symbols.

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