## Session "Molecules as Art ? Chair: Gabor Naray-Szabo

#### VISUALIZING THE UNSEEN

Paper presented at the Euroscience Open Forum, Stockholm on August 25, 2004

# W. Gerhard Pohl Austrian Chemical Society

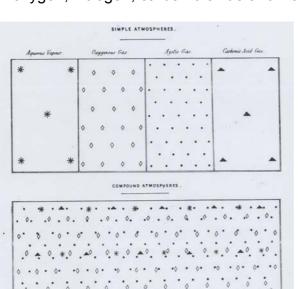
#### Introduction:

To introduce myself, I could say that I have four professions: chemist, teacher, historian and friend of the arts (if this can be called a profession). Therefore I will deal with my subject from four points of view. In the center of my considerations are atoms, molecules and their models.

## Development of models

The famous Austrian physicist Boltzmann wrote (quote): "...it is a strange desire of the human mind to build models and to try to improve them to get closer and closer to reality..."

Concerning the models of atoms this goes back to the Greek philosopher Democritus about 500 before Christ. The poet Lucretius about 100 before Christ made in a sense models of molecules when he said that smell is transferred by particles of different form, which fit into holes of the same form sitting in the skin of the smelling organ. In the middle ages, the high time of Alchemy, the microscopic view disappeared. Around 1800 John Dalton was the first to think about atoms as real particles, spheres of different size and weight. His representation of air as a mixture of molecules of oxygen, nitrogen, carbon dioxide and water vapour is only a symbolic picture (Fig.1)

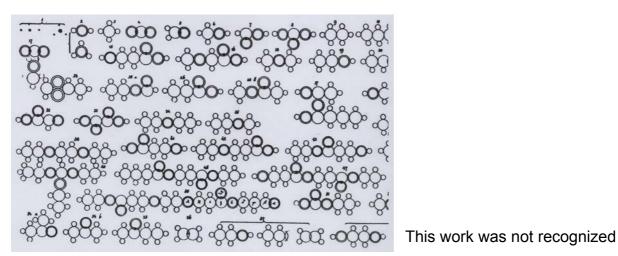


In 1811 Amadeo Avogadro clearly defined the difference between atoms and molecules. On the basis of his pioneering ideas the theory of gas kinetics was developed by Clausius, Maxwell and Meyer. Following their thoughts the Austrian scientist Josef Loschmidt (Fig. 2) imagined the real form of chemical molecules. In 1861, when he was still a teacher at a

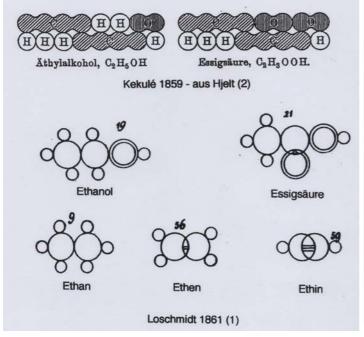
secondary school in Vienna, he published in his "Chemische Studien 1".

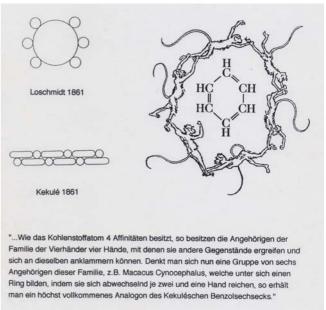


By geometrical reasoning he developed more than 300 formula of molecules in accordance with the chemical properties of the substances (Fig. 3)



by the famous chemists of his time, particularly August Kekule, who thought it was principally impossible to say anything about the real form of molecules. Later it turned out that Loschmidt's formula were far superior to Kekule's and resemble molecular models of today (Fig. 4 and 5).





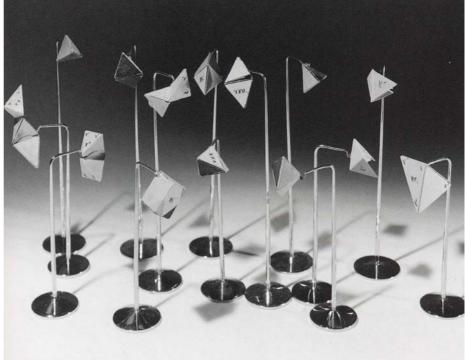
(von C.F.Findig "Zur Konstitution des Benzols", 1886)

Loschmidt was disappointed by the lack of recognition and turned into physics. In 1865 he calculated on the basis of the kinetic theory of gases the diameter of molecules of air (oxygen and nitrogen). His result, a diameter of about **one nanometer** for nitrogen is not far off the value known today. So in a way Loschmidt could be called the grandfather of the NANO-WORLD. He also calculated the number of molecules in one cubicmillimeter air. This number was called Loschmidt's number by Boltzmann. Today this name is not used any more, but was replaced by Avogadro's number, counting the molecules in 22,4 I gas (that is one mol).

Loschmidt's drawings remained twodimensional, they were projections of the molecules into a plane. Jacobus Hendricus van't Hoff in 1874 introduced three dimensions into molecular models. With the tetraedric arrangement of the four carbon-bonds (Fig. 6)

he explained many properties of organic molecules, which could not be understood before van't Hoff's work. He sent his paper-models to several famous chemists and found recognition by most of them. A group of these models looks like a work of "minimal art" (Fig. 7).



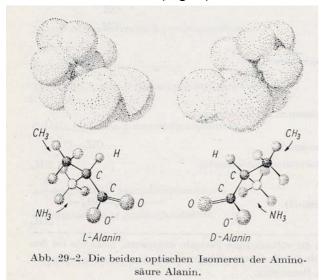


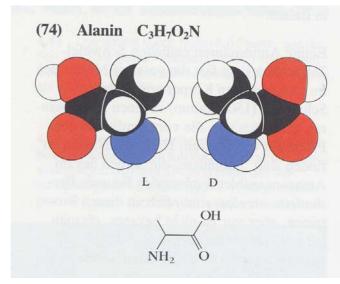
Van't Hoff did not only impress scientists. In a van't Hoff biography the Brasilian emperor Dom Pedro II is quoted asking at a visit in van't Hoff's laboratory in 1876 "..if it was possible to market the models as toys, to further early the chemical knowledge of children..."

### Verification of Models

Science made a quantum step after von Laue discovered X-ray scattering in 1912 and the Braggs developed the theory of X-ray scattering. Now the ideas of van't Hoff could be verified by experiments.

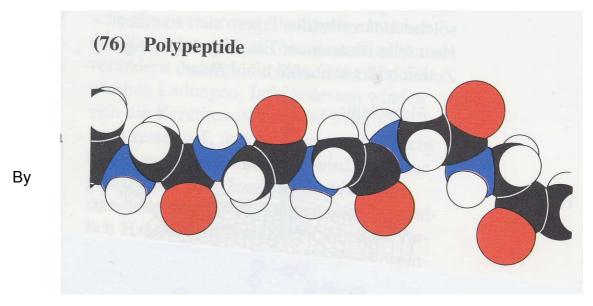
Between 1940 and 1950 Linus Pauling used X-ray scattering to develop his view of the chemical bond. In his "General Chemistry" which appeared in 1950 many molecular models as we know them today were drawn, like the L- and D-isomers of the aminoacid Alanin (Fig. 8).



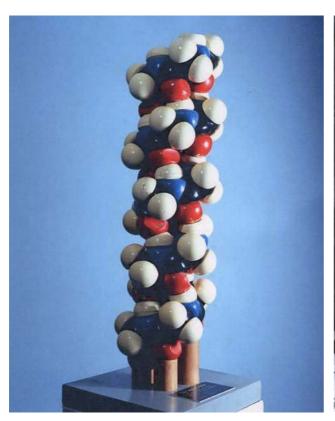


The drawing of Alanin was much improved by the illustrations of Peter Atkins book "Molecules" from 1988 (Fig. 9).

From the same book I took a beautiful presentation of a polypeptide chain (Fig. 10).



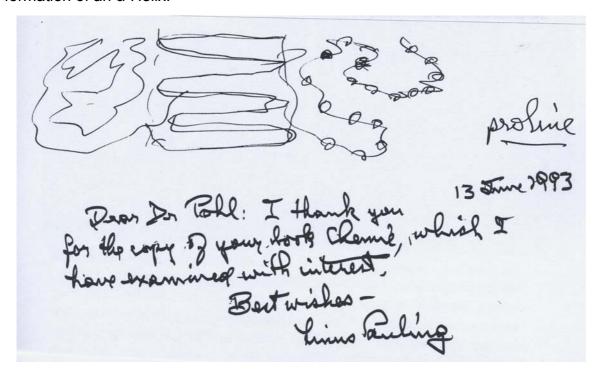
using X-ray data and model building Pauling and Corey found the famous  $\alpha$ -Helix in 1951. The model of the Helix really looks like the work of an artist (Fig. 11).





Linus Pauling was proud of having beaten Max Perutz and the Cambridge group in search for basic structures in proteins (Fig. 12).

I am proud of owning a drawing which was made by Pauling when I discussed with him the structure of proteins as a student (at the Lindau nobelist-meeting 1964) (Fig. 13). He mentioned that the aminoacid Proline for sterical reasons prevents the formation of an  $\alpha$ -Helix.



## Models in Teaching

Around 1960 the British nobel-prize-winner Sir George Porter emphasized the importance of molecular models to further the understanding of scientific ideas in the general public (quote) (Fig. 14)

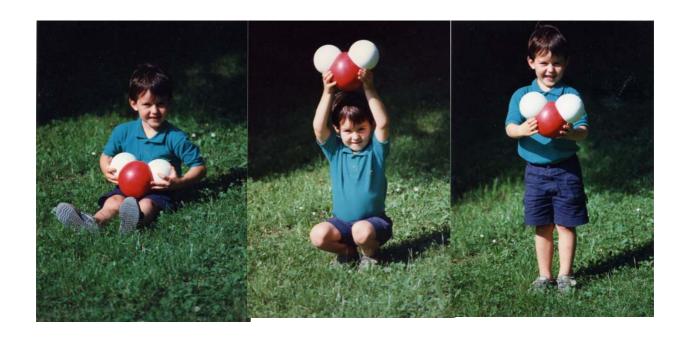
"The majority of people in this country still can't tell you the difference between an atom and a molecule..... They really ought to know about H, O, N and C and that they have 1, 2, 3 and 4 prongs. That's not much to ask of them.... Science is introduced into a child's experience far too late. CHILDREN OF FIVE should be exposed to science - they SHOULD PLAY WITH A MODEL OF H2O as soon as they play with a model of a crane." **ZITAT nach Sir George Porter** brit.Chemiker, geb. 6.12.1920 Nobelpreis für Chemie 1967 gemeinsam mit Manfred Eigen und Ronald G.W. Norrish

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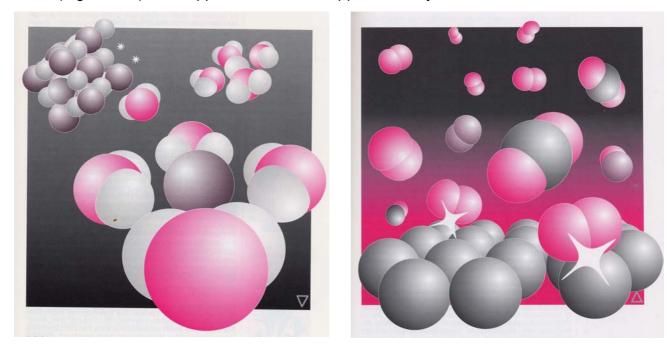
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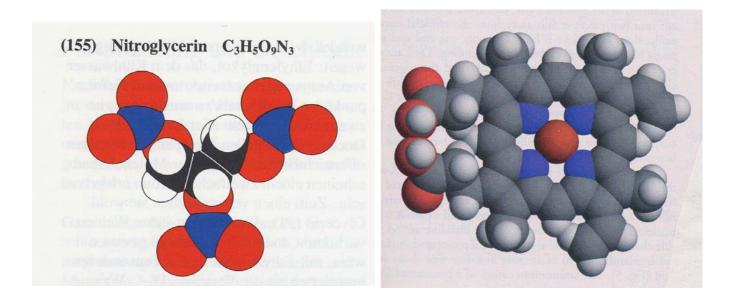
I tried to follow this suggestion of Sir Porter, made a threedimensional model of water and gave it to a five-year old son of a friend.(Fig. 15 a, b, c) He liked to play with it, but I don't know if this helped him to understand science better.



In my textbook "Chemie" first published in 1991 and with improved illustrations in 1998 I have used drawings of molecular models to give a vivid picture of the nanoworld (Fig. 16, 17). This approach has been appreciated by the students.

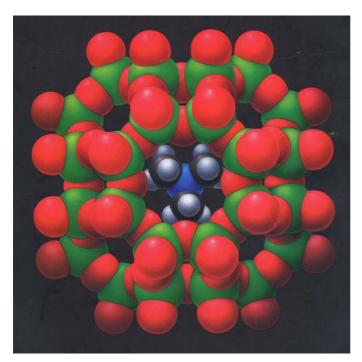


Nearing the end of my lecture I want to show a few other beautiful molecules. I want to mention Nitroglycerine (Fig. 18) because we are in Stockholm and this molecule was the basis of Alfred Nobel's fortune.

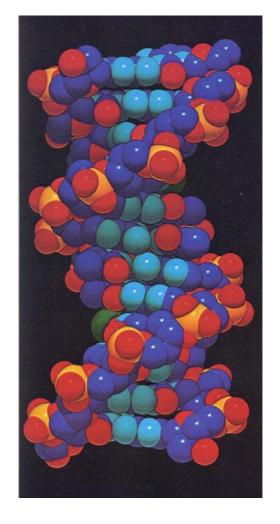


Heme (Fig. 29) is the oxygen-binding molecule in the center of hemoglobin, which is the basis for our life.

The Zeolite Rho (Fig. 20) is an active catalyst in the synthesis of methylamines. It retains the trimethylamine which is an unwanted by-product. In this case we see a little bit the connection between structure and function. Whereas mono- and dimethyl amines can leave the catalyst through the holes in its lattice, the size of trimethylamine is such that it cannot get out.



Many connections between structure and function have been clarified by molecular models in the case of enzymes and other proteins. Another famous model explains the way of identical reduplication of genetic information.



Let me end with the unusually coloured model of the famous B-DNA (Fig. 21), because one of the fathers of this most important molecular structure of the 20<sup>th</sup> century Francis Crick has passed away recently.

For this picture I want to quote the nobel-prize-winner Max Delbrück who said in 1979:

"...the whole business was like a child's toy that you could buy at a dime store, all built in this wonderful way that you could explain in LIFE-magazin so that really a five-year-old can understand what's going on....This was the greatest surprise for every one..."

Thank you!