

A short history of molecular modelling: 1860-1890.

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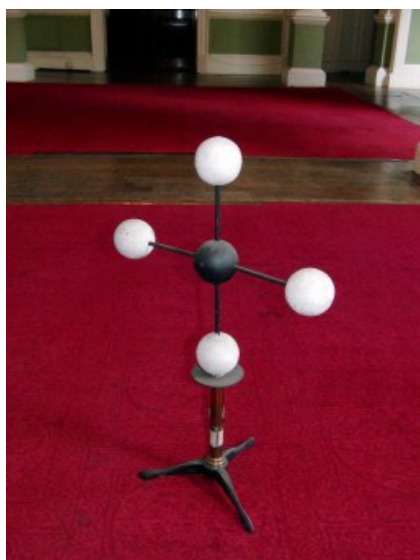
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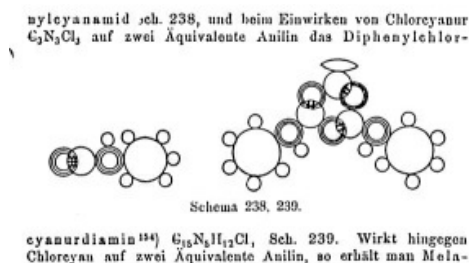
In 1953, the model of the DNA molecule led to what has become regarded as the most famous scientific diagram of the 20th century. It had all started 93 years earlier in 1860, at a time when the tetravalency of carbon was only just established (by William Odling) and the concept of atoms as real entities was to remain controversial for another 45 years (for example Faraday, perhaps the most famous scientist alive in 1860 did not believe atoms were real). So the idea of constructing a molecular model from atoms as the basis for understanding chemical behaviour was perhaps bolder than we might think. It is shown below, part of a set built for August Wilhelm von Hofmann as part of the lectures he delivered at the Royal College of Chemistry in London (now Imperial College).



The original August Wilhelm von Hofmann molecular model

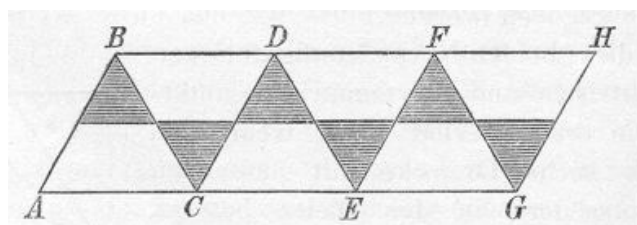
This grand-daddy of all molecular models does have some interesting features. The most obvious is that the carbon atom at the centre is square planar (tetrahedral carbon was still 14 years in the future). What HAS survived to the present day is the colour scheme used (black=carbon, white=hydrogen, and not shown here, red=oxygen, blue=nitrogen, green=chlorine). But another noteworthy aspect is the relative size of the white hydrogen, which is larger than the black carbon. This deficiency was however very soon rectified in 1861 by Josef Loschmidt, who published a famous pamphlet in which he set out his ideas for the structures of more than 270 molecules (many of which by the way were cyclic, and

this some four years before Kekule's dream!). An example (#239) is shown below, which gets the relative sizes of the atoms more or less correct (OK, chlorine is shown with rather an odd shape). To get an idea of how good Loschmidt's model actually was, click on the diagram to load a modern model, and compare the two! Even more impressive, these diagrams pre-date [van der Waals](#) work on the finite sizes of atoms, first presented in 1873.



Loschmidt's molecular models. Click for 3D

To conclude, I cannot resist showing one more model. [Hermann Sachse](#) believed cyclohexane could not be planar. To try to convince people, in 1890 he included a "flat-packed" model in the pages of a journal article, evidently believing that people would cut it out, and assemble it into a 3D shape.



Flat-packed molecular model of cyclohexane

You might have noticed a theme in the present blog of presenting 3D models for many of the molecules I discuss (include the Loschmidt one above). For the historians amongst you, I note our [1995 article](#) in which we updated[1] Sachse's origami with an article featuring how to incorporate interactive models into journals (still sadly only too rare). Perhaps a history of the molecular model, and how it has been presented over 150 years might be an interesting one to trace!

REFERENCES

1. O. Casher, G.K. Chandramohan, M.J. Hargreaves, C. Leach, P. Murray-Rust, H.S. Rzepa, R. Sayle, and B.J. Whitaker, "Hyperactive molecules and the World-Wide-Web information system", *J. Chem. Soc., Perkin Trans. 2*, pp. 7, 1995. <http://dx.doi.org/10.1039/P2995000007>