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A FAILED ENCOUNTER IN MATHEMATICS AND CHEMISTRY: THE FOLDED MODELS OF VAN ‘T HOFF AND SACHSE

Abstract: *Three-dimensional material models of molecules were used throughout the 19th century, either functioning as a mere representation or opening new epistemic horizons. In this paper, two case studies are examined: the 1875 models of van ‘t Hoff and the 1890 models of Sachse. What is unique in these two case studies is that both models were not only folded, but were also conceptualized mathematically. When viewed in light of the chemical research of that period not only were both of these aspects, considered in their singularity, exceptional, but also taken together may be thought of as a subversion of the way molecules were chemically investigated in the 19th century. Concentrating on this unique shared characteristic in the models of van ‘t Hoff and the models of Sachse, this paper deals with the shifts and displacements between their operational methods and existence: between their technical and epistemological aspects and the fact that they were folded, which was forgotten or simply ignored in the subsequent development of chemistry.*

Keywords: *folded and foldable models; stereochemistry; mathematization of chemistry; shifts in epistemological modi; van ‘t Hoff; Sachse*

Neúspěšné setkání matematiky a chemie: van ‘t Hoffovy a Sachsovy skládací modely

Abstrakt: *Trojrozměrné modely molekul bývaly užívány v průběhu celého 19. století jednak za účelem reprezentování, jednak se záměrem otevírání nových epistemických obzorů. V této studii jsou sledovány dva případy: van ‘t Hoffovy modely z roku 1875 a Sachsovy modely z roku 1890. Neobvyklost těchto dvou případů spočívá v tom, že v nich byly modely molekul nejen fyzicky skládány, ale také matematicky konceptualizovány. Ve světle chemického výzkumu příslušného období se ukazuje, že byly oba tyto aspekty výjimečné, a to každý zvlášť i v jejich propojení, které lze ve vztahu ke způsobu, jakým v 19. století chemický výzkum molekul probíhal, považovat za subversivní. Autor se v předložené studii zaměřuje na tento společný jmenovatel van ‘t Hoffových a Sachsových modelů, přičemž sleduje změny a posuny ve vztahu mezi jejich operativními metodami a jejich realizací, resp. mezi jejich technickými a epistemologickými aspekty na jedné straně a, na straně druhé, jejich materiálním sestrojením (pomocí skládání), které bude další rozvoj chemie přehlížet, pokud na ně jednoduše nezapomene.*

Klíčová slova: *skládané modely; stereochemie; matematizace chemie; změny v epistemologických modech; van ‘t Hoff; Sachse*

MICHAEL FRIEDMAN
Humboldt University, Excellence Cluster “Image Knowledge Gestaltung”
Interdisciplinary Laboratory Image Knowledge Gestaltung
Sophienstraße 22a, 10178 Berlin, Germany
email / michael.friedman@hu-berlin.de

Introduction

The role of three-dimensional models of molecules in chemistry, starting from mid 19th century – and especially the relations between the various physical models, the drawings in the various research papers and the chemical formulas – had a decisive importance and with it a long and intricate history.[1]

These models – being either iconic diagrams or material and three-dimensional, made from sticks and balls, wires, or cardboard – aimed at representing molecules, their shape or the spatial relations between different composing atoms. These models were not treated and approached by all of the chemists at that time in the same manner. Explicitly, they were treated either as having solely educational purposes, or as being a mere representation of molecules, or even as stimulating new experiments and predicting new, not-as-yet-observed results. The goal of this paper is to survey two unique episodes in the history of these material models of molecules, concentrating on models of molecules made from foldable cardboard: the 1875 models of Jacobus Henricus van ‘t Hoff and the 1890 models of Hermann Sachse.

As an epistemological framework, one may claim that the physical models of molecules oscillated in general between two modi of existence. Firstly they were treated as a mere representation of a molecule, thus having, for example, educational value and eventually considered as a technical object; secondly they operated and functioned epistemologically, as an epistemic thing – i.e. they hinted either at the existence of new molecules or at new

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[1] See for example: Eric FRANCOUER, “The Forgotten Tool: The Design and Use of Molecular Models.” *Social Studies of Science*, vol. 27, 1997, no. 1, pp. 7–40; Eric FRANCOUER, “Beyond Dematerialization and Inscription. Does the Materiality of Molecular Models Really Matter?” *HYLE. International Journal for Philosophy of Chemistry*, vol. 6, 2000, no. 1, pp. 63–84; Ursula KLEIN, “Techniques of Modeling and Paper Tools in Classical Chemistry.” In: MORGAN, M. S. – MORRISON, M. C. (eds.), *Models as Mediators*. Cambridge: Cambridge University Press 1999, pp. 146–167; Ursula KLEIN, *Experiments, Models, Paper Tools*. Stanford: Stanford University Press 2003; Christoph MEINEL, “Molecules and Croquet Balls.” In: DE CHADAREVIAN, S. – HOPWOOD, N. (eds.), *Models: The Third Dimension of Science*. Stanford: Stanford University Press 2004, pp. 242–275.

theories, concerning their spatial structure. In the latter case, however, these molecules (or the predications concerning them or their structure) were not (yet) observed via experiments in the laboratory.[2] Within this framework, folded models opened, as I aim to show, new epistemological horizons in stereochemistry, and their modi of existence varied between *three* poles: between being an epistemological thing, being a technical-representational model, and being completely forgotten.

But before turning into the detailed analysis of these models, I would like to briefly touch on the subject of stereochemistry, which deals with the relative spatial arrangement of atoms, and henceforth, with the structure of molecules.[3] As is well known today, two molecules, which are composed of the same elements but whose three-dimensional structure is different from each other, may have different physical and chemical properties. The intuitive example for two objects that may look identical to each other but have a different three-dimensional structure is the right hand compared to the left one. But it was only during the later 1840s and in the 1850s that the following conclusion was drawn, that the arrangement of atoms in space does matter and that this arrangement cannot be reduced to the identity and the number of the composing atoms. This was noted in 1848 by Louis Pasteur,[4] with his insight that there are two types of molecules of tartaric acid:[5] these must not only be three-dimensional but also defer with respect to this structure. It is van ‘t Hoff, however, who is considered the father of stereochemistry.

Both van ‘t Hoff and Sachse used folded models and both either derived mathematical constraints from them or derived models themselves from mathematical theory. In the works (and models) of their followers, however, such mathematization was either ignored along with the operation of folding or simply forgotten. The question that this paper intends to answer is

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[2] Here and throughout the paper, I follow the differentiation presented by Hans-Jörg Rheinberger between an epistemic thing and a technical object. See Hans-Jörg RHEINBERGER, *Toward a History of Epistemic Things. Synthesizing Proteins in the Test Tube*. Stanford: Stanford University Press 1997, and especially *ibid.*, pp. 28–31. See also Hans-Jörg Rheinberger’s paper in this volume.

[3] For an extensive analysis of the beginnings of stereochemistry, see Peter J. RAMBERG, *Chemical Structure, Spatial Arrangement: The Early History of Stereochemistry, 1874–1914*. Aldershot: Ashgate 2003.

[4] Louis PASTEUR, “Sur les relations qui peuvent exister entre la forme cristalline, la composition chimique et le sens de la polarisation rotatoire.” *Annales de Chimie et de Physique*, 3rd series, vol. 24, 1848, no. 6, pp. 442–459.

[5] Called today l-(+)-Tartaric Acid (or *dextrotartaric acid*) and d-(-)-Tartaric Acid (or *levotartaric acid*).

why these two interrelated aspects of representation were forgotten, whereas other methods of representation were preferred. In section 1 I review the work of van ‘t Hoff in the field of stereochemistry, in light of his folded models. Section 2 deals with the folded models of Sachse. I claim that while van ‘t Hoff’s models were epistemological at the beginning, afterwards they became technical, and their mathematical aspects were forgotten. By contrast, Sachse emphasized that his folded models stemmed from a mathematical theory; he thus pointed towards a possible (though partial) reduction of (stereo)chemistry to mathematics, which might have led to a rejection of his models. Section 3 therefore deals with this failed connection between folded models and mathematics.

1. Van ‘T Hoff Folds a Letter

In 1874, 26 years after Louis Pasteur’s insight, the chemist Jacobus Henricus van ‘t Hoff (1852–1911) published his celebrated manuscript *Voorstel tot Uitbreiding der Tegenwoordige in de Scheikunde gebruikte Structuurformules in de Ruimte*.[6] This publication, along with the almost simultaneous publication of Joseph Le Bel,[7] signified, together with Pasteur, the modern birth of stereochemistry. It was in this manuscript that van ‘t Hoff suggested that molecules have a three-dimensional structure.[8] More explicitly, van ‘t Hoff proposed that the four valencies of the carbon atom are directed towards the vertices of a tetrahedron. It is well known today – as was also known to van ‘t Hoff several years after the publication of his various manuscripts – that he was not the first to present and think of the carbon atom as a tetrahedron,

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[6] Jacobus H. van ‘t HOFF, *Voorstel tot Uitbreiding der tegenwoordig in de scheikunde gebruikte Structuur-Formules in de ruimte; benevens een daarmee samenhangende opmerkung omtrent het verband tusschen optisch actief Vermogen en Chemische Constitutie van Organische Verbindingen*, Utrecht 1874.

[7] Joseph Achille LE BEL, “Sur des relations qui existent entre les formules atomiques des corps organiques et le pouvoir rotatoire de leurs dissolutions.” *Bulletin de la Société chimique de France*, vol. 22, 1874, pp. 337–347. Note that Le Bel did not draw any models in his paper.

[8] Several models for representing molecules existed before and during the time of van ‘t Hoff’s models. Among these models, the most famous one is the Stick-and-Ball model of Kekulé, which had definitely influenced van ‘t Hoff. Other models were the croquet ball models of August Wilhelm Hofmann, the brass strip models of James Dewar or Crum Brown’s Structural Diagrams. All of these models, except Kekulé’s, were two-dimensional and were not intended to represent any three-dimensional molecular structure. See: MEINEL, “Molecules and Croquet Balls”.

where the carbon atom is located at its center.[9] Indeed, other chemists hinted that the existence of isomers is the result of three-dimensional structure. What van ‘t Hoff and his colleagues introduced in that period was a twist within the relation between the chemical, arbitrary, heuristic formulas and realistic interpretation, which consisted of considering the role of geometry, which I will discuss later. But although van ‘t Hoff’s ideas were already to some extent present in the 19th century chemistry community, it seems that, as Peter J. Ramberg describes, “van ‘t Hoff’s [...] 1874 Dutch pamphlet would suffer the [...] fate of obscurity, and chemists would learn of van ‘t Hoff’s ideas only through his extensively revised editions in French (*La chimie dans l’espace*, [published in] 1875) and in German (*Die Lagerung der Atome im Raume*, [published in] 1877).”[10] Here I would like to examine what role folded models played within the salvation of van ‘t Hoff’s discoveries from the “fate of obscurity”.

The initial manuscript of van ‘t Hoff and his 1874 translation into French *Sur les formules de structure dans l’espace*[11] included only written descriptions and figures. Van ‘t Hoff begins by comparing the possible number of isomers the carbon atom would have if it had been planar in contrast to what is known empirically. It is quite possible that he referred here to August Wilhelm Hofmann’s “glyptic” formulas.[12] In this way van ‘t Hoff reaches a conclusion that the number of isomers “is evidently a much greater number than those known so far.”[13] Van ‘t Hoff therefore proposes that a “second assumption brings theory and fact into agreement, that is, by imagining the affinities of the carbon atom directed towards the corners of a tetrahedron

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[9] For example, see Alan J. ROCKE, *Image and Reality: Kekulé, Kopp, and the Scientific Imagination*. Chicago: University of Chicago Press 2010, pp. 228–260. “[A]t least four other chemists explicitly invoked the carbon tetrahedron during the 1860s: Pasteur in 1860 [...], [Aleksandr] Butlerov in 1862, [Marc Antoine] Gaudin in 1865, and [Emmanuele] Paternò in 1869. [Johannes] Wislicenus stressed the need to consider three-dimensional spatial considerations for certain molecules at least three times before 1874.” (*ibid.*, p. 252). Thus, for example, Paternò “had [already] used the concept of a tetrahedral carbon atom for the explanation of a case of isomerism.” (*ibid.*, p. 251).

[10] RAMBERG, *Chemical Structure, Spatial Arrangement*, p. 53.

[11] Jacobus H. van ‘t HOFF, “Sur les formules de structure dans l’espace.” *Archives Néerlandaises des Sciences Exactes et Naturelles*, vol. 9, 1874, pp. 445–454.

[12] These “glyptic formulas” are in fact sculpted three-dimensional models of molecules made of croquet balls (representing atoms), connected by metal rods. However, these sculptures were in fact flat. See: MEINEL, “Molecules and Croquet Balls”, pp. 250–252.

[13] Peter J. RAMBERG – Geert J. SOMSEN, “The Young J. H. van ‘t Hoff: The Background to the Publication of his 1874 Pamphlet on the Tetrahedral Carbon Atom, Together with a New English Translation.” *Annals of Science*, vol. 58, 2001, p. 67 (51–74).

whose central point is the atom itself."[14] Turning the attention of the reader to two isomers of the molecule whose base formula would be $C(R_1R_2R_3R_4)$ (where the R_i might represent different groups, i.e. molecules that are bound to the carbon atom, denoted by C), he remarks that "in cases where the four affinities of the carbon atom are saturated with four mutually different univalent groups, two and not more than two different tetrahedra can be formed, which are each other's mirror images, but which cannot ever be imagined as covering each other, that is, we are faced with two isomeric structural formulae in space."[15] This is illustrated with two diagrams, to be found at the end of van 't Hoff's Dutch pamphlet (see diagrams *VII* and *VIII* in Figure 1).

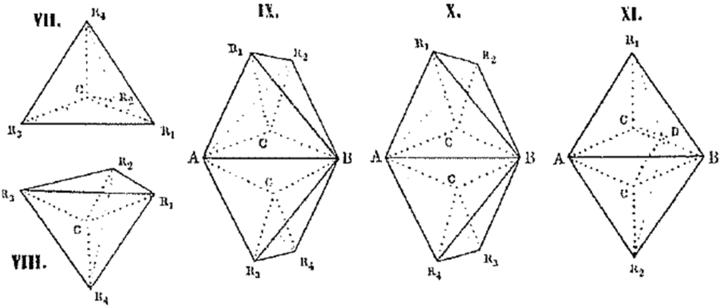

Figure 1: van 't Hoff figures (*VII–XI*) from *Voorstel.*[16]

With this representation, double bonds resp. triple bonds between two carbon atoms are represented through a common edge resp. a common face. However, as we will see, later versions (and also former contemplations) of van 't Hoff's manuscript show that he thought that double bonds could also be represented by attaching two tetrahedra at a vertex. The carbon atom itself was represented as the central point of the tetrahedron, denoted always by C. Using this suggested three-dimensional structure, van 't Hoff predicts new, not-yet found isomers, but still somewhat hesitates regarding the factual status of his new representation: "The difference between these figures, whose

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[14] *Ibid.*
[15] *Ibid.*, pp. 67–68.
[16] HOFF, *Voorstel*, fig. VII–XI.

number is limited to two, predicts a case isomerism that is not present in the older means of representation. Returning now to the facts, I believe that I have found examples of this isomerism among the organic compounds."[17]

However, as these pamphlets went almost unnoticed, in 1875 van 't Hoff published an extended version in French, *La chimie dans l'espace*, providing the reader with more illustrations and showing advancements in van 't Hoff's research.[18] Disregarding for a moment the footnotes in this manuscript, there is no hint whatsoever that when van 't Hoff refers to representation, as in the former manuscript, he refers to a drawn as well as to a *material*, folded representation. However, at the first footnote in the 1875 manuscript, van 't Hoff stresses the possibility that folded, colored cardboard models would be sent to the reader upon his wish: "There may be some difficulty in following my reasoning; I felt it myself, and I have used models [*figures*] of cardboard to facilitate the representation."[19] In addition, he mailed these models to the leading chemists at that time, but these were not considered as an essential part to the text – van 't Hoff still referred mainly to the drawings at the end of the papers and manuscripts and the models from cardboard are mentioned only in the footnotes. Moreover, it is not clear, from taking a look at the models in Figure 2 whether it is essential that they be folded out of cardboard and not be prepared from other materials; I will return to this point later.

Figure 2: Van 't Hoff's 1875 models as presented in Museum Boerhaave, Leiden.[20]

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[17] RAMBERG – SOMSEN, "The Young J. H. van 't Hoff," p. 71.

[18] Jacobus H. van 't HOFF, *La chimie dans l'espace*. Rotterdam: Bazendijk 1875.

[19] *Ibid*., p. 7, footnote 1: "Il y aura peut-être quelque difficulté à suivre mon raisonnement; je l'ai senti moi-même, et je me suis servi de figures en carton pour faciliter la représentation."

[20] Copyright: Museum Boerhaave, Leiden (Inventory num.: V 10239).

An extensive description of van ‘t Hoff’s models is given by Trienke M. van der Spek.[21] It is important nevertheless to emphasize that the models enabled van ‘t Hoff to show the tetrahedron as what enables molecular asymmetry, when such tetrahedra were also irregular.[22] Indeed, referring to a set of models being made between 1875 and 1877, van der Spek notes that “[t]hese models illustrate van ‘t Hoff’s deeper understanding that an asymmetric tetrahedron – rather than a regular one – most adequately represents the asymmetry of a carbon atom surrounded by four different groups.”[23]

What is already remarkable in these models is that the carbon atom is nowhere to be found – locating the center of the tetrahedron, as the presumed location of the carbon atom, is left to the reader. As will become eventually clear in the 1877 version of the *Voorstel*, van ‘t Hoff is not interested in where the carbon atom *is*, but rather in the *spatial relations* between different atoms and molecular groups. Moreover, as was already noted,[24] the models represent the spatial relations in two ways: the bound groups to the carbon are represented either by the faces or by the vertices, where the two representations are equivalent.

Indeed, the differences between the *Voorstel* and *La chimie dans l’espace* in the way van ‘t Hoff has proposed modeling and visualizing the three-dimensional structure of molecules are significant, but in 1877 – the year when the translation to German was published (*Die Lagerung der Atome im Raume*) – another major difference can be detected. Van ‘t Hoff did not send his models anymore, but rather wrote in an appendix a manual, proposing that the reader fold the models him/herself.

Mathematics and the Models In “Die Lagerung”

As is well known van ‘t Hoff was not only influenced by the traditions of structural chemistry in Bonn and Paris, but also by the emphasis put on

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[21] Trienke M. van der SPEK, “Selling a Theory: The Role of Molecular Models in J. H. van ‘t Hoff’s Stereochemistry Theory.” *Annals of Science*, vol. 63, 2006, no. 2, pp. 157–177.

[22] ROCKE, *Image and Reality*, p. 254: “[V]an ’t Hoff proposed in 1874 that molecular asymmetry, thus nonsuperposability, is established only by the *chemical* distinguishability of the four *geometrically indistinguishable* vertices of the regular tetrahedron.” (emphasis in original).

[23] SPEK, “Selling a Theory,” p. 163.

[24] *Ibid*., p. 166 and Bertrand O. RAMSAY, “Molecular Models in the Early Development of Stereochemistry. I: The van ‘t Hoff Model; II: The Kekule Models and the Baeyer Strain Theory.” In: RAMSAY, B. O. (ed.), *Van ‘t Hoff-Le Bel Centennial*. Washington, DC: American Chemical Society 1975, p. 77 (74–96).

mathematical studies and geometry at the University of Leiden.[25] Hence, it is not surprising to find that the appendix contains not only folding instructions, but also points towards the mathematical nature of the models. Indeed, the translator of *Die Lagerung*, Felix Hermann, suggests in a letter to van ‘t Hoff from 9 November 1875 that the mathematical background should be explained more extensively: “[...] it occurred to me on study of your work, that it could be made somewhat more palatable for the chemical public, for whom your theory is primarily intended. Developments of a mathematical nature, which for an audience trained in this area are easily comprehensible with only fleeting clues, must be recast explicitly to achieve the full understanding of a readership deficient in mathematical preparation who only rarely consider mathematical thoughts.”[26] Hermann’s approach also echoed van ‘t Hoff’s: according to van ‘t Hoff, the folded models gave organic chemistry a more geometrical and mathematical foundation, as we will see further.

The appendix of *Die Lagerung* starts with the following passage: “To facilitate the presentation, it is necessary to bring the figures directly to *visual perception* [directen *Anschauung*] through models. In the following figures the *nets* of the figures in question are drawn. These are best cut out of moderately thick cardboard. The dotted lines should be scored lightly with a sharp penknife. By folding along the scored lines, the figure is spatially brought together and held together by gluing the side-mounted cutouts at the inner side of the space.”[27]

Two aspects in this opening passage are apparent: the material one and the mathematical one. Concerning materiality, what is clear here is that the action of folding is necessary for the understanding of van ‘t Hoff’s novel conception of stereochemistry: one must fold the cardboard and glue it in order to have a direct *Anschauung*.

Where did this idea of folding come from? The idea is first presented in a letter van ‘t Hoff sent to Gustav Bremer in December 1874, where one can detect a precursor to the folded models.[28] In this letter van ‘t Hoff attempted to explain the spatial structure of the two different isomers of tartaric acid,

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[25] See RAMBERG – SOMSEN, “The Young J. H. van ‘t Hoff,” p. 55.

[26] RAMBERG, *Chemical Structure, Spatial Arrangement*, p. 358. See also *ibid.*, p. 86, indicating that also Hermann was “mathematically inclined”, as Wislicenus described him.

[27] Jacobus H. van ‘t HOFF, *Die Lagerung der Atome im Raume*. Braunschweig: Vieweg 1877, p. 46 (emphasis added).

[28] The letter is published in: W. P. JORISSEN, “Eenige brieven van Van ‘t Hoff (1874–1875).” *Chemisch Weekblad*, vol. 21, 1924, no. 43, pp. 495–497 (495–501). See also SPEK, “Selling

whose chemical (basic) formula is $C_4H_6O_6$, and two of the isomers of Erythritol, whose chemical formula is $C_4H_{10}O_4$. A figure in the letter depicts two rows, consisting of four congruent triangles, above and below a line denoted by AB, where the faces of the triangles are painted either with white, gray or black. Columns I and III (see Figure 3.(1)) are associated to the two isomers of the tartaric acid, where the white, grey and black *faces* correspond to the molecular groups H, OH and CO_2H; columns II and IV are associated to two isomers of Erythritol (now called L-(-)-threitol and D-(+)-threitol), where the white, grey and black *faces* correspond to the molecular groups H, OH and CH_2OH. Folding along the line AB gives rise to the two isomers of tartaric acid (with columns I and III) and the two isomers of Erythritol (with columns II and IV).[29] Indeed, in the middle of every triangle a carbon atom is located; once one folds along the line AB, the two carbon atoms are to be imagined as bonded together, with a bond that is not depicted in any form (see Figure 3.(2)). The folding enables the "connecting" of the two "parts" of the molecules; however, one must note here that the two triangles cannot exist first on their own (as the carbon atom has valence four, but is connected in the "first stage" – i.e. before the folding – only to three groups in each triangle), when only afterwards the two carbon atoms bond with each other. Van 't Hoff is of course aware of this, but does not mention it in his letter.

The fold is considered as a tool to illustrate the structure of isomers, but not as what represents the process of the emergence of these molecules in reality. Moreover, it seems that van 't Hoff has taken into consideration this epistemological problematic, that the models imply, but could not eliminate it completely. Although later models do show the final form (as we saw above), van 't Hoff does give instructions how to fold his models, as we will see later. However, it is obvious that this folding – either with the folding of the letter or with the folding of the models – does not aim to represent how molecules are formed.

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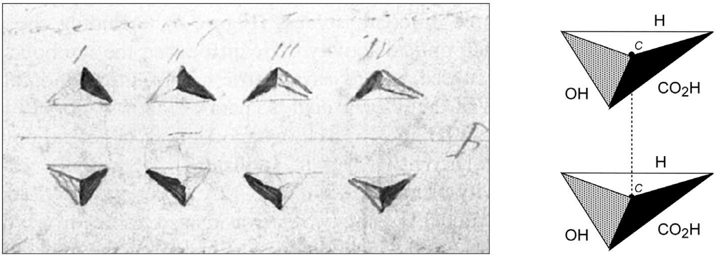
a Theory," p. 165; E. FISCHMANN, "A Reconstruction of the First Experiments in Stereochemistry." *Janus*, vol. 72, 1985, pp. 131–156.

[29] Van 't Hoff wrote the following to Bremer: "Stellen de drie driehoekjes in een der grootere, wit, ≡ en zwart, de groepen H, OH en CO_2H voor, in 't geval van Erythit H, OH en CH_2OH, zoo komt men tot de 4 denkbare isomeren, als men de figuur langs AB dubbel omvouwt, zoodat de driehoekjes twee aan twee op elkaat vallen" (in JORISSEN, "Eenige brieven van Van 't Hoff," p. 496).



(1) (2)

Figure 3: (1) Van 't Hoff's first attempt to model the isomers via a folded model.[30] (2) The result of folding the two triangles (in column I) one on top on the other, creating one of the isomers of the tartaric acid (figure drawn by M. F.).

It is clear that this letter represents a preliminary stage in van 't Hoff's conception of the three-dimensional structure of molecules. He does not mention the tetrahedron as the three-dimensional form of the carbon-atom, and moreover there is a lack of experimental data, with which one can verify the different structures. But already here one can detect two crucial aspects: firstly – considering the later versions of the manuscripts of van 't Hoff – that either the faces or the vertices could represent the different groups of molecules; secondly, that the triangles are not regular, i.e. isomers should not be necessarily represented by regular polygons or polyhedra. However, the instruction to actually fold a piece of paper or cardboard was omitted from the *Voorstel* and its subsequent versions, and reappeared only in *Die Lagerung*. Let me now return to the appendix of *Die Lagerung*. As was mentioned above, besides the material aspect, a mathematical aspect is also present, already in the first paragraph. This is revealed via the word *Netze*, that is, a net of a polyhedron. Van 't Hoff did not use this expression in the earlier versions, as he did not need it – there were no nets there to fold. Moreover, as we will see, this is not the only mathematical aspect.

The appendix then gives instructions on how to fold several nets, proposing that the models would be either face-centered or vertex-centered in order to illustrate the different isomers (see Figure 4). And while figures 39 till 49 of *Die Lagerung* depict models composed of equilateral triangles, the

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[30] Taken from: *ibid*.

models drawn in figures 55 till 63 do not have to be composed of these triangles: several models are composed of different, non-equilateral triangles.

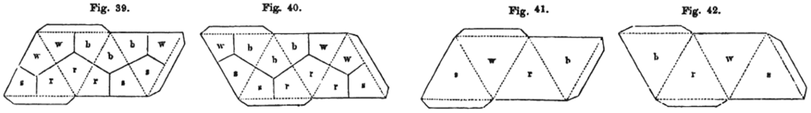

Figure 4: Figures 39–40 from *Die Lagerung*: vertex-centered models, figures 41–42: face-centered models.[31]

In which way folding was essential to van ‘t Hoff’s conception is to be seen in the following remark regarding the nets presented in Figure 5.(a): “If one assembles the net in such a way that one time the upper side, the other time the lower side would be the outer face of the resulting figure, the result is two mirror imaged tetrahedra representing two isomers [...].”[32] Explicitly, the resulting isomers (and how they are constructed) are induced from the action of folding. Moreover, using the unfolded nets, van ‘t Hoff can make several restrictions regarding the models themselves. Denoting by *a* and *b* the lengths of two of the edges of the triangles in figure 55 in *Die Lagerung* (see Figure 5.(b)), van ‘t Hoff notes[33] that *b* is dependent on *a* such that the following inequality results: $\frac{\sqrt{3}}{6}a < b$. For other models van ‘t Hoff supplied other inequalities and restrictions regarding the lengths of their edges; he did not, however, provide any proof, regarding such geometrical reasoning, according to which these restrictions could be considered true. Moreover, this raises another epistemological difficulty: van ‘t Hoff does not indicate what do these mathematical restrictions actually mean regarding the physical spatial structure of the molecule involved, i.e. what, if any, are the derived physical characteristics of the molecules which are represented by these polyhedra. Although it is clear that these are instructions on how to draw and construct the different models, van ‘t Hoff does not mention their explicit relation to physical reality or how these restrictions might be disco-

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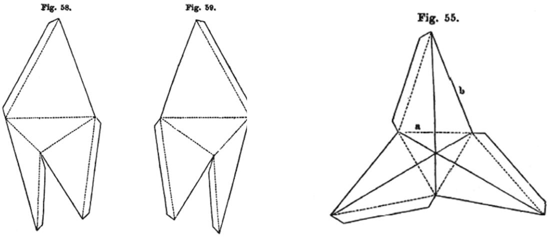
[31] HOFF, *Die Lagerung der Atome im Raume*, p. 47.

[32] *Ibid.*, p. 52: “Wenn man das Netz in der Weise zusammenfügt, dass einmal die obere Seite, das andere Mal die untere Seite zur Außenfläche der entstehenden Figur wird, so erhält man zwei enantiomorphe Tetraeder, welche die beiden Isomeren der oben erwähnten Combination darstellen.”

[33] *Ibid.*, p. 50.

vered or empirically proved via experiments in the laboratory. Moreover, as was mentioned before, van ‘t Hoff did not intend to imply that the folding of the molecules is a realistic depiction of a process taking place in reality (starting from a planar form and then being folded, due to other chemical processes) – but this was to some extent implied from the model itself. In addition, although the first models of van ‘t Hoff consisted of regular tetrahedra, the models presented at the appendix are irregular.



(a) (b)

Figure 5: (a) Two models of van ‘t Hoff, showing the dependence of the suggested molecule on the way folding is done, (b) Figure 55 from van ‘t Hoff’s *Die Lagerung* by means of which van ‘t Hoff exemplified a dependence on the mathematics.[34]

Van ‘t Hoff worked within a tradition where models were used for educational purposes. However, Van ‘t Hoff’s “important innovation [was] that his models were [...] meant to mimic directly certain physical characteristics of the molecule.”[35] But one has to ask what is meant here by “mimicry”: the fold indeed manifests clearly that van ‘t Hoff’s interest was in the spatial and geometrical relations between atoms and not in where the atoms themselves were or what the structure of the atom was. However, the explicit mathematization of these relations, which was only implicit in the earlier versions, reveals also the epistemological problem – i.e. problematizing the relations of these models to reality itself – and hence made the models into an epistemic object rather than a technical one. In this sense the models were not only educational, but also hinted towards other epistemological horizons, which not only consisted of discovering new isomers, but also of possible chemical constraints stemming from mathematics.

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[34] *Ibid.*, p. 52, 50.

[35] RAMBERG, *Chemical Structure, Spatial Arrangement*, p. 85.

After 1877: The Disappearance of the Fold

This epistemological tension is somewhat resolved – or better formulated, ignored or left aside – in the following years and in van ‘t Hoff’s subsequent publications regarding this subject. It is important to note that by 1878 van ‘t Hoff was a professor of Chemistry, Mineralogy, and Geology at University of Amsterdam. As a result he may not have had the time or the need to continue sending his models, as his proposal regarding the structure of the carbon atom was accepted and disseminated by other scientists. In addition, almost all of his publications after that year dealt with other subjects.

Moreover, when considering subsequent editions of *La Chimie dans l’espace* or of *Die Lagerung*, it seems that van ‘t Hoff had chosen to overlook the epistemological difficulties hinted at above, as one can hardly find a trace of folded models or of the action of folding itself. In 1887, van ‘t Hoff published *Dix années dans l’histoire d’une théorie*, subtitled as a second edition of *La chimie dans l’espace*. This manuscript contains the main arguments of his theory together with an historical account, along with the inclusion of new experiments and theories, which had taken place since 1877. Compared to *La chimie dans l’espace*, *Dix années* refers only once to models in a subsection entitled *Représentation graphique:* “To understand the difference between the two groups in question one can make use of two tetrahedrons made of cardboard, cut and pasted based on the Fig. 6 and 7; the four different groups supposed at the vertices of the tetrahedra are indicated by colors [...].”[36] The figures 6 and 7, to which van ‘t Hoff refers to, are shown in Figure 6:

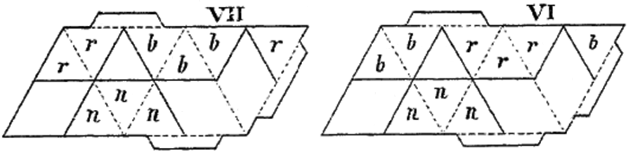

Figure 6: Figures 6 and 7 from Dix années dans l’histoire d’une théorie.[37]

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[36] Jacobus H″.van ‘t HOFF, *Dix années dans l’histoire d’une théorie.* Rotterdam: Bazendijk 1887, pp. 26–27: “Pour bien saisir la différence des deux groupements dont il s’agit on peut faire usage de deux tétraèdres en carton, coupés et collés d’après les Fig. 6 et 7; les quatre groups différents supposés aux sommets des tétraèdres sont indiqués par des couleurs [...]”.

[37] *Ibid.*, plates VI–VII.

This near-disappearance of the folding of the models is to be seen most clearly in 1894, when the second edition of *Die Lagerung* was published. This extended version, spans over more than 130 pages, and contains the now famous figures of the tetrahedron model for the carbon atom. Van ‘t Hoff mentioned his models only briefly: “For an explanation of the factual situation by the model one can use the tetrahedron made of cardboard, in which the various groups are elucidated by gluing the little caps of the colored paper [...].”[38] Van ’t Hoff also mentioned his models several other times,[39] however, there was no drawing of how the tetrahedron should be folded (as in *Dix années*) and no elaborate explanation of the different options for folding in the second 1894 edition of *Die Lagerung*.

Moreover, together with the disappearance of the folding of the models in van ‘t Hoff writings, it is to be noted that while numerous manuscripts and chemists relied on van ‘t Hoff explicit models of the tetrahedron,[40] they only took the final form of it – i.e. the two dimensional drawing of the three-dimensional tetrahedron. Wislicenus, in his paper *Über die räumliche Anordnung der Atome in organischen Molekülen und ihre Bestimmung in geometrisch-isomeren ungesättigten Verbindungen*, used the van ‘t Hoff’s model,[41] but drew neither the carbon atom nor the valence lines. Moreover, in 1890 Hantzsch and Werner took van ‘t Hoff’s idea one-step further. Researching the stereochemistry of nitrogen, they used a model that resembled van ‘t Hoff’s tetrahedron, but the nitrogen was placed at a vertex and the edges illustrated the lines of valence (see Figure 7).

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[38] Jacobus H. van ‘t HOFF, *Die Lagerung der Atome im Raume*. 2nd ed., Braunschweig: Vieweg 1894, p. 6: “Zur Erläuterung der Sachlage durch das Modell kann man sich der Tetraeder aus Pappe bedienen, bei denen die verschiedenen Gruppen durch angeklebte Käppchen aus farbigem Papier erläutert werden [...].”

[39] *Ibid.*, p. 37, 38.

[40] For the acceptance of van ‘t Hoff’s models, see e.g. RAMBERG, *Chemical Structure, Spatial Arrangement*, chap. 4, and Peter J. RAMBERG, “Pragmatism, Belief, and Reduction. Stereoformulas and Atomic Models in Early Stereochemistry.” *HYLE. International Journal for Philosophy of Chemistry*, vol. 6, 2000, no. 1, pp. 35–61.

[41] Johannes WISLICENUS, “Über die räumliche Anordnung der Atome in organischen Molekülen und ihre Bestimmung in geometrisch-isomeren ungesättigten Verbindungen.” *Des. XIV. Bandes der Abhandlungen der mathematisch-physischen Classe der Königl. Sächsischen Gesellschaft der Wissenschaften*, vol. 14, 1887, pp. 12–13, 16 (1–77).

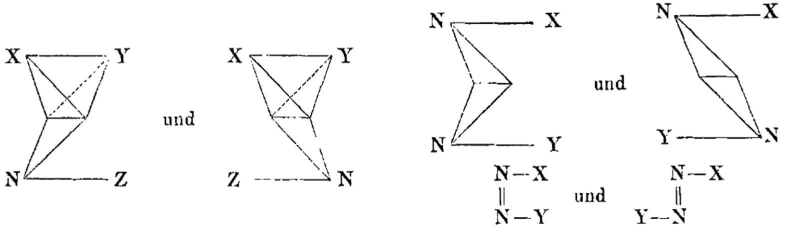

Figure 7: Isomers with nitrogen according to Hantzsch and Werner.[42]

With the model of Hantzsch and Werner it is easy to see that they do not think any more in terms of a folded model, since the four figures they had drawn (see Figure 7 above) contain edges, which are not the edges of a polygon, depicted either by the N-Z bond (left) or by the N-Y bond (right). The Hantzsch and Werner's models are, one might say, a hybrid of van 't Hoff's three-dimensional folded models, where the faces themselves may also represent the groups connected to the central atom, and Kekulé's Ball and Stick model, where the balls represent the atoms and the sticks represent the valence lines. But even if one does consider this model a hybrid, this points also to the dematerialization of the (folded) models, since the haptic property of the van 't Hoff models no longer existed in these examples. Formulated in other terms, the iconic dimension of these drawings and models became more dominant.

As Ramberg notes, the "stereoformulas that literally depict a polyhedron are physically and chemically curious, because they de-emphasize the bonding relationships, and include edges of the polyhedra which have no physical or chemical significance."[43] But not only that – already with the passage to Hantzsch and Werner's models it should be noted that van 't Hoff's model ignores the position of the carbon atom. Whereas the other models attempt to generalize van 't Hoff's they are forced to revise the tetrahedron model, which results in free-floating edges,[44] therefore no longer indicating their spatial arrangement. To that one might add that the mathematical

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[42] Arthur HANTZSCH – Alfred WERNER, "Über die räumliche Anordnung der Atome in stickstoffhaltigen Molekülen." *Berichte der deutschen Chemische Gesellschaft*, vol. 23, 1890, p. 19 (11–30).

[43] RAMBERG, "Pragmatism, Belief, and Reduction," p. 39.

[44] Indeed, all the three edges coming out of the nitrogen atom in Figure 7 are on the same plane.

constraints, which van ‘t Hoff material models imposed on the physical structure of the molecule, notwithstanding their ambiguous, unclear status, were now completely ignored.

It might be suggested that van ‘t Hoff’s folded models served as an *epistemological procedure* – they pointed towards a knowledge that was not yet determined (to be noticed in the attempted mathematization), and highlight a discipline in the process of becoming, that isstereochemistry. However, the disappearance of folding – taking only the end product (tetrahedron) – and its replacement by more iconic diagrams designate the replacement of this epistemological procedure by a technical object. The action of the folding of the models was gradually forgotten or disappeared, while the final form of the model was preferred. What resulted from this partial, gradual disappearance is the hybrid form, resembling more a three-dimensional variant of Kekulé’s models. With this in mind, I turn now to another example of the intersection of mathematics and folded models in chemistry – that of Hermann Sachse.

2. Hermann Sachse’s Three Equations

Hermann Sachse’s (1862–1893) explanation for the three-dimensional structure of benzene, having C_6H_6 as the molecular formula, and for the cyclohexane rings (hexamethylene), having C_6H_{12} as the molecular formula, could be seen as another attempt to use the van ‘t Hoff’s tetrahedron model for other molecules, and this was indeed Sachse’s motivation. However, it is worth examining Sachse’s articles in more detail. Since Sachse also indicated that his models should be folded, he also took the relations between mathematics and chemistry more seriously.

In 1888 Sachse suggested a stereochemical model of the benzene molecule, which was compatible with Kekulé’s suggested structure. Sachse referred to a physical model, demanding that the reader follows his descriptions, as (two-dimensional) figures and drawing would be too complex, on the one hand, and that even the clearest description of the spatial relations would be no replacement for a model, on the other.[45] By that Sachse empha-

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[45] Hermann SACHSE, “Über die Configuration des Benzolmoleküls.” *Berichte der deutschen Chemische Gesellschaft*, vol. 21, 1888, p. 2531, footnote 2 (2530–2538): “Da selbst die klarste Beschreibung dieser räumlichen Verhältnisse keinen genügenden Ersatz eines Modelles zu bieten vermag, Zeichnungen andererseits höchst complicirt ausfallen würden, so ist im Interesse möglichster Kürze alles folgende unter der Voraussetzung dargestellt, dass der geehrte Leser die weiteren Erörterungen durchweg am Modell verfolgt.”

sized the advantages that haptic, three-dimensional models could have in comparison to a visual, graphic, i.e. to iconic two-dimensional models, or to a mere description – although at this point (i.e. with the 1888 paper) it is not clear what is meant by the "clearest description", since, as we will see further, other scriptural-mathematical methods would later also serve Sachse to explain his results. Sachse's model for the benzene molecule consisted of taking a cardboard model of an octahedron, removing two parallel triangular faces and gluing on the six remaining faces a regular tetrahedron.[46] In 1890 Sachse took his 1888 open-ended octahedron as motivation for modeling the isomers of cyclohexane.

Before dealing with Sachse's paper from 1890, I would like to make a detour and turn to what was believed, during the 1880s, as the three-dimensional structure for molecules with molecular formula C_nH_{2n} where $n > 1$, and in particular – for the cyclohexane (whose formula is C_6H_{12}). The three-dimensional structure of the ring of the carbon atoms of these molecules was believed to be a flat ring. Therefore Johann Friedrich Wilhelm Adolf von Baeyer (1835–1917) believed the cyclohexane to be flat, i.e. it was regarded as a having a planar hexagonal shape. Based on the experimental results between benzene and cyclohexane,[47] Baeyer published in 1885 his research regarding the spatial structure of the above-mentioned molecules. Since benzene had, as was proved by Kekulé, a spatial structure, where all the carbon atoms were on the same plane, it seems that Baeyer wanted to implement the same conclusion on molecules of the form C_nH_{2n}. Indeed, Baeyer[48] suggested that there is a strain in the molecule, i.e. a strain that happens when a molecule forms angles that are abnormal. By this Baeyer meant that while the normal, i.e. regular "tetrahedral" valence angle of carbon is 109^0,28' (i.e. the angle between the two lines, where each line connects a different vertex of a regular tetrahedron with its center), every deviation from that value would cause strain, eventually resulting in a given molecule's instability. What Beayer proposed is to model these molecules together with the strain that is caused by the abnormal angle via Kekulé's ball and stick models, suggesting that the sticks could be bent: "One can easily have an idea of the meaning of this sentence [regarding the normal angle 109^0,28'

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[46] *Ibid.*, p. 2532. Sachse does not even supply a drawing in this paper, and gives the reader – in a contrast to his own objection! – a mere description of how to build the model. However, in his paper from 1890 Sachse does give a drawing of his model (see Figure 9).

[47] See RAMSAY, "Molecular Models in the Early Development of Stereochemistry," p. 91.

[48] Adolf von BAEYER, "Ueber Polyacetylenverbindungen. Zweite Mittheilung." *Berichte der Deutschen Chemischen Gesellschaft*, vol. 18, 1885, pp. 2269–2281.

and the strain], by taking into account the ball model of Kekulé, and assuming, that the wires of a resilient spring are movable in a similar way in all directions."[49] Baeyer supplied a figure then, depicting how the different rings ought to look (see Figure 8) and what the corresponding deviation should be.

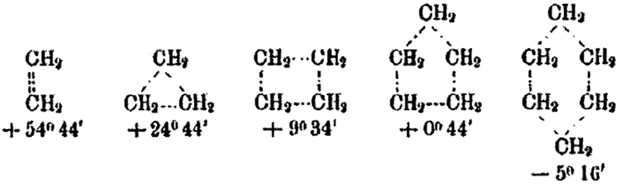

Figure 8: Baeyer's two-dimensional depictions[50] of molecular rings of the form C_nH_{2n} for the values $n = 2, \ldots, 6$.

Needless to say, Baeyer's concrete choice of the physical model might have also implied his own understanding of the spatial structure of these molecules. Concerning the molecule C_6H_{12}, Baeyer's assumption led to the conclusion that the valence angles in the cyclohexane ring would deviate (from the angle 109^0,28'), causing a strain in the molecule, as a planar configuration would have valence angles of 120^0. What goes unmentioned is the very suggestion of an option that this tension might be relieved or would not even exist due to another, three-dimensional configuration of the carbon-atoms.

However, Sachse had another structure in mind. In 1890 he suggested that the cyclohexane rings could be strain-free, i.e. the normal valence angle 109^0,28' could be maintained, as the carbons have no need of lying on a single plane.[51] He proposed two non-planar models for the cyclohexane, call-

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[49] *Ibid.*, p. 2278: "Eine Vorstellung von der Bedeutung dieses Satzes [regarding the 109^0,28' normal angle] kann man sich leicht machen, wenn man von dem Kekulé'schen Kugelmodel ausgeht, und annimmt, dass die Drähte, einer elastischen Feder ähnlich, nach allen Richtungen hin beweglich sind."

[50] *Ibid.*, p. 2279.

[51] The planar structure for the carbon atoms that Baeyer proposed for the molecules C_4H_8 and C_5H_{10} was also wrong: i.e. the ring of the carbon atoms of both of these molecules is non-planar. For C_4H_8 the ring of carbon atoms has a folded or "puckered" conformation, and for C_5H_{10} the ring has an unstable puckered shape that fluctuates. The ring of carbons for C_3H_6 is planar, but this molecule is highly unstable. Note the molecule propene has the same chemical formula as C_3H_6 but is non-planar, hence these two molecules are isomers.

ing them "symmetric" (now known as the *chair model*) and "asymmetric" (known as the *boat model*). How did Sachse construct his models? Both of the models were constructed via *folding* a piece (or two pieces) of cardboard into an open ended octahedron (resp. into two octahedra), and then attaching tetrahdra on certain dark triangles, drawn inside the faces of these folded cardboard pieces (see Figure 9 and 10). The first three-dimensional structure obtained is called "symmetrical" and the second "asymmetrical".

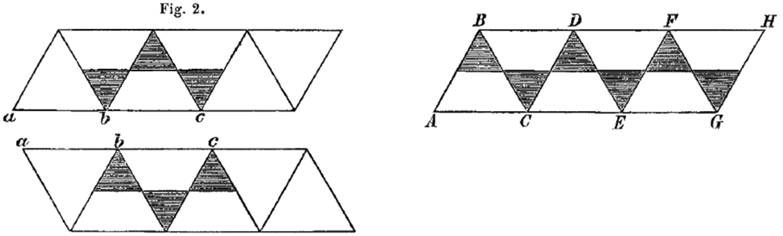

Figure 9: Sachse's 1890 cardboard models (before the folding) for the "asymmetrical" (left) and for the "symmetrical" (right) isomers of the cyclohexane.[52]

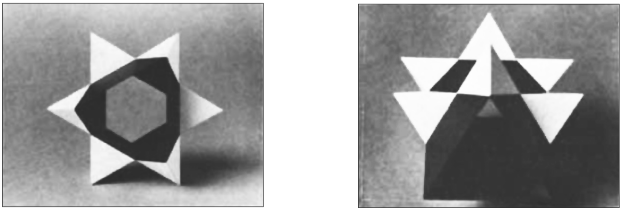

Figure 10: Colin A. Russel's modeling[53] of Sachse's two models: above: the "symmetrical", below: the "asymmetrical".

By using these physical models Sachse noted that one of the asymmetric models could be converted into the symmetrical one and vice versa, but only

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[52] Hermann SACHSE, "Über die geometrischen Isomerien der Hexamethylenederivate." *Berichte der deutschen chemische Gesellschaft*, vol. 23, 1890, p. 1366 (1363–1370).

[53] Colin A. RUSSELL, "The Origins of Conformational Analysis." In: RAMSAY, O. B. (ed.), *Van 't Hoff-Le Bel Centennial*. Washington, DC: American Chemical Society 1975, p. 175 (159–178).

after overcoming a certain resistance.[54] The physical models required pressure for this passage between the symmetric and asymmetric models. Sachse remarked that his models enabled this to be seen in the most convenient way.[55] However, in Sachse's 1890 paper one can already note a difference between his approach and van 't Hoff's regarding the way mathematics relates to the folded models. While van 't Hoff's approach, although being ambiguous, derived mathematical properties from models, Sachse declared, relating the task of finding the three-dimensional structure of the cyclohexane, that: "For solving this problem, which leads to a system of three equations, there are two different configurations. Fortunately, these configurations have the same geometric properties, which allow visualization [Veranschaulichung] of these systems by easily produced models."[56] The folded models are presented instead by the three equations to enable the visualization. These equations are not even presented in the 1890 paper, and according to Sachse are not derived from the physical models. However, it seems that the mathematical analysis was not only done before producing these models, but was in fact preferred by Sachse.

This can be seen all the more clearly with Sachse's 1892 paper. Trying to better explain the arguments leading him to claim the existence of the two isomers, the 1892 paper contains the complete mathematical analysis.[57] At the beginning of the paper Sachse presents a mathematical explanation, in order to explain why a configuration of a ring with six carbon atoms without strain is *mathematically* possible, when taking the regular tetrahedron model as representational.[58] The arguments that Sachse used are taken from the domains of geometry, trigonometry and calculus. After investigating molecular rings with fewer carbon atoms and proving the main mathematical claims, Sachse presented the three equations, which were announced two years before.[59] Solving these equations, a calculation that spans over six

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[54] SACHSE, "Über die geometrischen Isomerien der Hexamethylenederivate," p. 1368: "Es ist also dabei stets ein gewisser Widerstand zu überwinden."

[55] *Ibid.*, p. 1368, footnote 1: "Für unser Modell wurde die am leichtesten darstellbare Phase gewählt."

[56] *Ibid.*, p. 1365: "Aus der Lösung dieser Aufgabe, welche zu einem System von 3 Gleichungen führt, ergeben sich zwei verschiedene Configurationen. Glücklicherweise haben dieselben gewisse geometrische Eigenschaften, welche eine Veranschaulichung dieser Systeme durch bequem herzustellende Modelle gestatten."

[57] Hermann SACHSE, "Über die Konfigurationen der Polymethylenringe." *Zeitschrift für physikalische Chemie*, vol. 10, 1892, pp. 228–241 (203–241).

[58] See *ibid.*, p. 209.

[59] *Ibid.*, p. 231.

pages, proved the *mathematical* existence of the desired three-dimensional structures – the symmetric and the asymmetric one. The passage from the asymmetrical one, described as more unstable, to the symmetric model, was also described mathematically. However, towards the end of the paper Sachse remarked that it was with the folded model that one could detect more clearly the resistance encountered when the transition from the asymmetric to the symmetric isomer occurred.[60] Sachse concluded his paper with a rather pungent remark, stating that since Baeyer no longer allowed the "language of models" when dealing with rings with six carbons, he assumed that such a ring must be planar.[61]

Although Sachse's died in 1893, his contribution was not totally ignored; it was, however, by and large rejected.[62] Thus, for example, in 1893, Arthur Hantzsch noted in his *Grundriss der Stereochemie* the two predicted isomers, but formulated these in terms of planar rings, repeating Baeyer's arguments verbatim.[63] Although Hantzsch did not refer to any of Sachse's proposed models, it seems that he implicitly hinted at the use of such models. Hantzsch indicated that the strain in the molecules of the form C_nH_{2n} "can be presented graphically through situated symbols", referring to page 93 in his book.[64] On this page one can find a figure, which in fact might have resembled Sachse's models, were Hantzsch not convinced of the validity of Baeyer's arguments (see Figure 11).

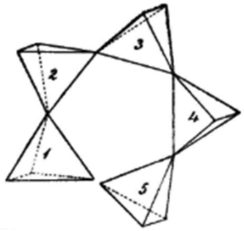

Figure 11: Hantzsch's drawing for the Pentane molecule C_5H_{12}, when he uses the van 't Hoff's model, i.e. where every tetrahedron represents a carbon atom, where the non-bounded vertices represent hydrogen atoms. Hantzsch indicates that: "[...] if the configuration of such paraffins is illustrated by the tetrahedral theory, for Pentane the symbols are obtained [as in the figure.]"[65]

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[60] See *ibid.*, p. 238.

[61] *Ibid.*, p. 241. It is not clear whether by "models" Sachse refers to Kekulé's examples, since on the one hand Sachse (in this passage) also talked about Kekulé's "Kugelmodelle" (i.e. the ball and stick models), and on the other, as we saw, Baeyer was familiar with Kekulé's models. It might be that Sachse referred to his own models.

[62] See RUSSELL, "The Origins of Conformational Analysis," pp. 164–169.

[63] See Arthur HANTZSCH, *Grundriss der Stereochemie*. Breslau: E. Trewendt 1893, p. 98.

[64] *Ibid.*, p. 97: "Diese Verhältnisse lassen sich auch durch die auf pag. 93 befindlichen Symbole anschaulich darstellen."

[65] *Ibid.*, p. 93.

As is well known, it was Ernst Mohr who revived Sachse's theory in 1918, in his paper *Die Baeyersche Spannungstheorie und die Struktur des Diamanten*,[66] which resurrected and elaborated on Sachse's work. As the title of Mohr's paper indicates, he analyzed diamonds, and using the X-ray diffraction as proposed by Bragg in 1913[67] he showed that Sachse's chair conformation is the basis for the structure of the diamond. However, the main point for our discussion is that Mohr used completely other physical models than Sachse to visualize the way these molecules are arranged in space, as can be seen in Figure 12:

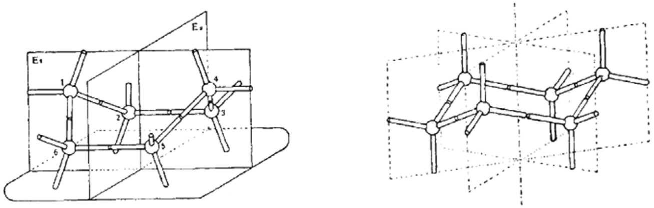

Abb. 1. Abb. 3.

Figure 12: Mohr's two models for the cyclohexane (left – the asymmetric, right – the symmetric).[68]

Mohr's explanation as to the rejection of Sachse's model was that there was no experimental confirmation to his predictions.[69] This of course changed at the time Mohr wrote his paper (although the final experimental proof was given in the 1950s by Barton et al.[70]). However, as one can clearly see, Mohr does not only abandon the folded models of Sachse regarding the molecule C_6H_{12}, but also hardly mentioned the latter's theoretical-mathe-

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[66] Ernst MOHR, "Die Baeyersche Spannungstheorie und die Struktur des Diamanten." *Journal für Praktische Chemie*, vol. 98, 1918, no. 1, pp. 315–353.

[67] The crystal structure of diamond was the first crystal structure to be determined by X-ray diffraction. This was published in 1913 by William Lawrence Bragg and his father William Henry Bragg (see: William H. BRAGG – William L. BRAGG, "The Reflection of X-Rays by Crystals." *Proceedings of the Royal Society of London, Series A*, vol. 88, 1913, no. 605, pp. 428–438).

[68] *Ibid.*, p. 317, 316.

[69] *Ibid.*, p. 318.

[70] See RUSSELL, "The Origins of Conformational Analysis," p. 164.

matical analysis.[71] In fact, the only instance when folded models appeared in the paper, they are presented as a "very approximated model"[72] of his ball and stick examples. Describing the three-dimensional structure of rings of an even number of carbon atoms in an unstrained position, Mohr first presented his own way of modeling the molecule C_8H_{16} (see Figure 13), i.e. a ring consisting of eight carbon atoms, and only then instructs on how to fold a cardboard model, gluing on the upper and lower triangles tetrahedral. Moreover, Mohr noted that in order to attach the tetrahedra "exactly on the right position"[73] to obtain an exact representation, one had to glue an underlay of a certain thickness on the upper resp. lower corner *P* of the triangles (see Figure 13). However, Mohr nowhere mentioned Sachse's very similar way of modeling, although he was certainly familiar with it.

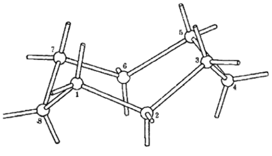
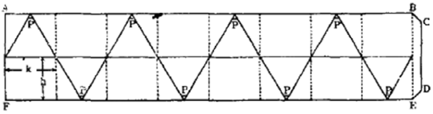


Abb. 23.



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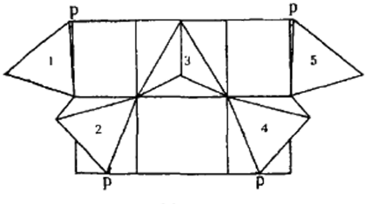

Abb. 25.

Figure 13: Mohr's ways of modeling a ring consisting of 8 carbon atoms. This configuration today is called the crown conformation of cyclooctane (also known as chair-chair); it was unknown in 1918 that the molecule C_8H_{16} has two additional arrangements (i.e. isomers): the chair-boat and the boat-boat arrangements.

3. Conclusion: Folded Models and Mathematics – a Failed Encounter

The reasons for the rejection of Sachse's theory are well documented. Not only was there a lack in experimental results, which could verify this model,

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[71] The 1892 paper of Sachse is mentioned only once; see: MOHR, "Die Baeyersche Spannungstheorie," p. 316, footnote 1.

[72] *Ibid.*, p. 351.

[73] *Ibid.*

but also the reputation associated with the theory and with the name of Baeyer certainly casts its shadow on the reception of Sachse's theory. Collin A. Russel describes several other reasons for this rejection: the status of scientific theory, the organization of the different fields of science[74] and more important to our discussion – the scientific communication through models. As Russel claims, the folded models "failed to demonstrate rotational effect"[75] and hence it is no surprise that Mohr replaced these models with his models.[76] Moreover, although Sachse was well aware of van ‘t Hoff's tetrahedron, he did not adopt his "Public Relation" methods of spreading his models (or was simply unaware of them) – i.e. in opposition to van ‘t Hoff, Sachse neither sent his models to his colleagues nor drew any figures of how these three-dimensional molecules would look like. In that sense, what was supposed to be a three-dimensional haptic model remained for Sachse a two-dimensional figure, whereas van ‘t Hoff emphasized the three-dimensional aspect more. In addition, whereas van ‘t Hoff made the separation between the two-dimensional drawing and the three-dimensional models, Sachse demanded from his reader to cut the paper they were reading and fold it. Explicitly, by asking to treat the paper as what should be essentially cut and folded and not just read, he demanded a reconsideration of how the medium transmits knowledge and added another layer of maneuverability to the "paper tools" themselves,[77] which was uncommon during that period.

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[74] RUSSELL, "The Origins of Conformational Analysis," pp. 170–175.

[75] *Ibid.*, p. 175.

[76] Interestingly, the mathematical community at the end of the 19th century was able to produce more advanced and more accurate (mathematical) material models, which could have demonstrated the desired "rotational effects", which the chemical models were aspiring to show. Examples of such models are to be found in the catalog of Walther von Dyck's exhibition in Munich in 1893; see Walter v. DYCK, *Katalog mathematischer und mathematisch-physikalischer Modelle, Apparate und Instrumente*. München 1893, reprint: Hildesheim: Georg Olms Verlag 1994. Contrary to chemistry, mathematical-material models were more abundant; starting from the middle of the 19th century till the 1920s, a golden age of mathematical model-production was taking place. See Anja SATTELMACHER, "Geordnete Verhältnisse. Mathematische Anschauungsmodelle im frühen 20. Jahrhundert." *Berichte zur Wissenschaftsgeschichte. Sonderheft ‘Bildtatsachen’*, vol. 36, 2013, no. 4, pp. 294–312; Herbert MEHRTENS, "Mathematical Models." In: DE CHADAREVIAN, S. – HOPWOOD, N. (eds.), *Models: The Third Dimension of Science*. Stanford: Stanford University Press 2004, pp. 276–306.

[77] See KLEIN, *Experiments, Models, Paper Tools*, p. 246: "[T]he syntax of paper tools – their visual form, rules of construction and combination, maneuverability – shapes scientists' production of chains of representation [...] formula equations came into the fore as a means of justification."

Notwithstanding these cultural and scientific aspects, the attempt to mathematize the folded models either by deriving them from mathematical properties (van 't Hoff) or by replacing them with a mathematical proof (Sachse), indicating that the three-dimensional structures of the molecules can be induced only via a geometrical-trigonometric theoretic reasoning, failed. It might be claimed that the consideration of mathematics within the already existing tension between the chemical reality – represented by the chemical formulas (as symbolic inscription as well as iconographic one[78]), perspective drawings and the hand-held models[79] – and the physical reality, made yet another twist in this relation, whose epistemological implications were simply rejected. This mathematization may be thought of as a later development in the conception of the Berzelian formulas, which were considered by Berzelius himself in 1814 as algebraic: explicitly, these chemical formulas he used were to be thought "*as* is done in algebraic formulas."[80] In contrast, for van 't Hoff, as well as for Sachse, several of the considerations and the arguments *were* simply mathematical.[81]

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[78] *Ibid.*, pp. 23–35.

[79] Cf. FRANCOUER, "Beyond dematerialization and inscription."

[80] Jöns J. BERZELIUS, "Essay on the Cause of Chemical Proportions, and on Some Circumstances Relating to Them: Together with a Short and Easy Method of Expressing Them." *Annals of Philosophy*, vol. 3, 1814, p. 52 (51–62) (emphasis added). Jacob Berzelius (1779–1848) is one of the founders of modern chemistry. As Klein describes, "[c]hemical formulas, such as H_2O for water or H_2SO_4 for sulfuric acid, were introduced in 1813 by [...] Berzelius." (KLEIN, *Experiments, Models, Paper Tools*, p. 2). See Klein's book for the epistemological consequences of the Berzelian formulas.

[81] Regarding the relation of chemists to mathematical arguments, see RAMBERG, *Chemical Structure, Spatial Arrangement*, p. 112, where Wislicenus is described as considering "Van 't Hoff's theory of the asymmetric carbon atom a fully justified mathematical expansion of our chemical views"; and pp. 189–191, concerning Victor Meyer; Meyer "oscillated between advocating the reduction of chemical theory to mathematical physics and then advocating its theoretical autonomy" (*ibid.*, p. 189). See also Mary Jo NYE, "Physics and Chemistry: Commensurate or Incommensurate Sciences?" In: NYE, M. J. – RICHARDS, J. L. – STUEWER, R. H. (eds.), *The Invention of Physical Science: Intersections of Mathematics, Theology and Natural Philosophy since the Seventeenth Century*. Dordrecht: Kluwer 1992, pp. 205–224. It is also noticeable that during the second half of the 19th century, mathematicians from England (e.g. J. J. Sylverster) emphasized the relations between chemistry and mathematics while relying on results from invariant theory. See Karen V. H. PARSHALL, "Chemistry through Invariant Theory? James Joseph Sylvester's Mathematization of the Atomic Theory." In: THEERMAN, P. – PARSHALL, K. V. H. (eds.), *Experiencing Nature: Proceedings of a Conference in Honor of Allen G. Debus*. The Western Ontario Series in Philosophy of Science, vol. 58, 1997, pp. 81–111.

While van ‘t Hoff’s mathematical considerations were easy to follow, and entailed no direct ontological claim regarding the structure of molecules, Sachse’s analysis, using for example differential calculus of functions with several variables and trigonometry, not only was not part of the tool-box of organic chemistry at the end of the 19th century, but also entailed the existence and non-existence of several three-dimensional structures. Moreover, while the theoretical models (such as the berzelian-symbolical ones) and the material models could motivate further experiments to prove or disprove the existence of what was predicted via these symbolic apparatuses, mathematical reasoning would imply the replacement of these models and eventually the reduction of chemistry to mathematical based physical laws. It might be suggested that Sachse himself was afraid of that problematic. Although in 1890 he already knew of the three equations that imply the non-planar structure of the cyclohexane, he chose to present his folded models instead.

However, Sachse changed his mind regarding this problematic. In 1892 he turned to what his theory was truly based upon: mathematics, stating that the physical, hand-held models imply certain special properties that arise from the models themselves.[82] The hand-held models can be manipulated – and the results of this manipulation might indicate properties, which eventually might not be true: i.e. although they transmit another type of knowledge and can be epistemologically productive, they can also be misleading. The replacement of the folded models by mathematics was not accidental, it was not just another way to explain the possible three-dimensional structures of cyclohexane. The replacement suggested that the folded models were implying properties that could be neither verified nor proved (neither by experiments nor by mathematics), properties that were associated uniquely to the models themselves. Therefore, in the 1892 work, Sachse declared that a “safe advancement in these areas is only possible if one limits himself to a step by step [investigation] regarding the necessary assumptions, and accordingly attempts to determine every theorem, conditions which are indeed indispensable.”[83] Needless to say, Sachse’s remark here echoes the by

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[82] SACHSE, “Über die Konfigurationen der Polymethylenringe,” p. 203: “Lässt man, wie es bisher geschehen, die Resultate gelten, die man erhält, wenn man die bekannten Kekuléschen Kugelmodelle zu Ringen zu vereinigen sucht, so legt man damit – bewusst oder unbewusst – gewisse spezielle Eigenschaften, die den Modellen anhaften, den Atomen bei.”

[83] *Ibid.*: “Ein sicheres Vorwärtsschreiten in diesen Gebieten ist nur dann möglich, wenn man Schritt für Schritt sich auf dies notwendige Maß der Annahmen beschränkt, und demgemäß für ein jedes Theorem festzustellen sucht, welche Voraussetzungen es zu wirklich unumgänglichen Bedingungen hat.”

then growing movement of axiomatization in mathematics and especially in geometry. In a word, Sachse's formulation greatly resembled mathematical reasoning, where it was required to prove rigorously every claim and to avoid redundant assumptions. In that sense, although Sachse's folded models could have been seen as complementary to mathematical 'paper-tools', they may have hinted – according the Sachse – towards other properties, which were redundant, i.e. which could not be proven or built upon. This is also indicated in the opening passage of Sachse's 1893 paper *Deutung der Affinität*. It was there that he remarked that "the language of mechanics will ultimately dissolve the language of our science."[84] This stands in stark contrast to Van 't Hoff's models, which were in some sense a means to end, serving at the beginning as an epistemological procedure (when van 't Hoff did try to mathematize them or at least to derive mathematical-chemical constraints out of them), but then shifted to a technical object, considered eventually and only as an end-product (the tetrahedron). Recalling Hans-Jörg Rheinberger's distinction between the "epistemic thing" and the "technical object",[85] one can see with van 't Hoff's models that the shift is gradual, and within this process certain characteristics are forgotten or abandoned. By contrast, Sachse's folded models were neither mathematized by him nor presented as technical objects, but rather chosen to be forgotten[86] and be completely *replaced* by a mathematical analysis. Implying that chemical research should be like mathematical research or even based or replaced by it possibly hinted at a subversion in the discipline of chemistry itself, causing Sachse's epistemological models to be rejected; hence they came to a dead-end and disappeared for more than 25 years.

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[84] "[...] [Die] Sprache der Mechanik [...], in die sich ja die Sprache unserer Wissenschaft schliesslich auflösen soll." In: Hermann SACHSE, "Eine Deutung der Affinität." *Zeitschrift für physikalische Chemie*, vol. 11, 1893, p. 185 (185–219). Cf. also the discussion in RAMBERG, *Chemical Structure, Spatial Arrangement*, pp. 188–191, on Meyer's hope regarding the understanding of chemical phenomena in terms of mathematical termini.

[85] RHEINBERGER, *Toward a History of Epistemic Things*, pp. 28–29.

[86] Cf. FRANCOUER, "The Forgotten Tool."