THE TOYS OF ORGANIC CHEMISTRY: MATERIAL MANIPULATIVES AND SCIENTIFIC REASONING

Abstract: *Chemical visualizations and models are special kinds of media for thinking. In this paper, I examine several historical case studies—an archive of images from museums, special collections, and popular magazines—as examples of emergent practices of physical modeling as theoretical play which became the basis for molecular biology and structural chemistry. I trace a legacy of visualization tools that starts with Archibald Scott Cooper and Friedrich Kekulé in the late 1800s, crystallizes as material manipulatives in Van't Hoff and his folded paper "toys," is legitimized in the California lab of Linus Pauling, and is glorified in the popular imaginary with James Watson and Francis Crick's model of DNA. My tracing then follows several threads into contemporary modeling practices. I ultimately argue that modeling play, originally outside of the boundary of deductive, positivist science, is now an accepted mode of reasoning in these related chemical fields.*

Keywords: *epistemology; manipulative models; materiality; toys in science*

Hračky organické chemie: materiální manipulativy a vědecké uvažování

Abstrakt: *Chemické vizualizace a modely jsou zvláštními druhy médií myšlení. Tato studie zkoumá několik historických případových studií – archív obrazů z muzeí, specializovaných sbírek a populárně-vědeckých časopisů – emergentních praktik materiálního modelování coby teoretické hry, jež se staly základem molekulární biologie a strukturní chemie. Sleduji dědictví nástrojů vizualizace počínaje Archibaldem Scottem Cooperem a Friedrichem Kekulé na konci 19. století, jejich vyústění do materiálních manipulativů Van't Hoffa a užití jeho skládaných papírových „hraček" Linusem Paulingem i jejich následné pronikání do populární obraznosti díky modelu DNA Jamese Watsona a Francise Cricka. Sleduji dále jejich vliv na současné praktiky modelování a zdůrazňuji, že materiální modely, jež tradičně stály za hranicemi deduktivní, pozitivistické vědy, jsou nyní v těchto oblastech chemie akceptovány jako způsob vědeckého uvažování.*

Klíčová slova: *epistemologie; manipulativní modely; materialita; hračky ve vědě*

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Introduction

In an iconic image of Nobel Prize winners James Watson and Francis Crick, the pair pose with their famous model, a spiral staircase made of delicate metal pieces. Crick gestures to the model, while Watson looks up. The men are young and unequivocally triumphant; the image thinly disguises its subjects' smugness, their slightly arrogant attitude towards their artificial poses. Historians have made much of the personalities of these two: unconventional, flippant, perhaps immature, and most certainly playful. The popular mythology that has developed around them would have us believe that they were boys playing with toys. But a critical consideration of epistemology in action must recognize that those were some pretty powerful toys. What is that model made of? How did they decide to put it together, and, more importantly who (or what episteme) taught him (or them) to do it? How did "playing with toys" come to be recognized as Nobel-worthy science?

Evelyn Fox Keller's book *The Century of the Gene* tells the story of the conceptualization of the gene—the irreducible unit of molecular biology—as a myth of simplicity that contemporary genetics is still struggling to escape with more robust and complex explanations. The crux of her criticism is the biologist's linguistic tools for representation and argumentation; the gene as a name and unit, she argues, has "simplicity and allure," but the tests of such a simple catch-all (gene as code and gene as driving action) have not born out. Keller ultimately claims, among other things, that "biologists who seek to make sense of [new developments in epigenetics and the like] will have a considerably expanded array of conceptual tools with which to work."[1] In a related version of the history of the gene, Philip Thurtle traces the cultural forces behind what he calls a "genetic rationality".[2] His argument focuses on the intersection of technologies and political ideologies[3] that animated the 20th century's uptake of the encoded "living material" approach to inheritance, eugenics, population and, more broadly, a genetic way of seeing life itself.

Though both of these approaches touch upon what I might call material and visual rhetorics, they really focus on the verbal and conceptual

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[1] Evelyn Fox KELLER, *The Century of the Gene*. Cambridge: Harvard University Press 2000, p. 10.

[2] Philip THURTLE, *The Emergence of Genetic Rationality*. Seattle: University of Washington Press 2007.

[3] Thurtle is less concerned with an "internalist" view of epistemology (as I am here), but rather with how knowledge functions as power in society large.

aspects of explanation and argumentation. But the epistemic practices of molecular biology and structural chemistry are often dependent upon embodied, material and spatial conceptualization; they require understanding of molecular architecture that natural spoken languages are ill-equipped to manage. Much of what scientists in these fields do is manipulate material (a model) which ostensibly represents the thing-in-itself (a molecule). Such epistemic work may be discursive, certainly, on one level, but its materiality calls for a different sort of frame with which to describe it. Keller's request for new "conceptual tools" for geneticists begs, from the historian, a detailed understanding of the conceptual tools that have existed to this point, a materialist media history of things we think with. Historians and philosophers of science—and particularly those who wish to treat structural chemistry, molecular biology, genetics and the like—must become historians and philosophers of media and technology.

The pages that follow are an example of a project to that end. In them, I briefly examine a few of the practices of physical modeling in organic chemistry that enabled the kind of material-theoretical play that, in turn, enabled James Watson and Francis Crick to conceptualize DNA and the modern world at large to conceive of the material replication of life as a primarily structural-chemical affordance. First, in a brief review of scholarly literature, I describe some current conversations in science studies that such a tracing might inform. Then I historicize the development of what Linus Pauling calls "spatial models" in molecular biology. My story isn't an unbroken historical line; it is rather an archaeology – a series of related snapshots, starting with the simultaneous innovation of drawing the valence structures of organic compounds by Archibald Scott Cooper and Friedrich Kekulé in the late 1800s. I trace those innovative visualizations into the toylike manipulatives used in labs like Linus Pauling's – the concepts made concrete that afforded the paradigm-establishing, now-iconic "model," then into the generally accepted, public scientific way of knowing as evidenced by mass-produced modeling kits that were sold as toys and used as pedagogical tools. Ultimately I'll argue, from the perspective of media theory, that the unique affordances of what I call "material manipulatives" – the tinkertoys of Linus Pauling's spatial models –were as important to the discovery of DNA's structure as the social and rhetorical situations that have already been so thoroughly historicized. The ongoing contemporary remediations of such methods also imply that the chemical spatial model persists as part of a now-unquestioned, arguably "invisible", epistemic practice in molecular biology.

Studies of inscriptions, visualizations, and modeling technologies in science

In an entry for the 2012 edition of the Stanford Encyclopedia of Philosophy, philosopher of science John Carroll lists discursivity as a point to be addressed in future scholarship; "more attention," he writes, "needs to be paid to the language used to report what are the laws and the language used to express the laws themselves."[4] I maintain that the equation, the diagram, and the manipulative are a material parallel to that language that is as powerful, or more powerful, than the verbal. Rhetoricians Alan Gross, D. S. Birdsell and L. Groarke would likely agree with Carroll's call to pay attention to inscription. Birdsell and Groarke hit upon the philosopher's "propositionality" and the relationship of the real to the representation of the real when they argue that scientific demonstrations "are inherently propositional because a visual image is used to convey information that is purportedly true."[5] In 2009, Gross wrote "Toward a Theory of Verbal-visual Interaction: The Example of Lavoisier", [6] in which, among other things, he calls for visual and material rhetorics of scientific arguments; he claims that much of science's convincing is done with meaningful images and objects, not words. Gross is careful to distinguish between the "verbal" kind of visualization – images that are symbolic and meaning-bearing, and the mimetic image – a photograph that is seen as empirical evidence in itself. He spends most of his time on the latter, and mimetic images are indeed inscriptions that require their own set of problematic rhetorical questions.

But I am more interested in what he has to say about the former – the more consciously signifying visualization tools. Gross maintains, most notably, that visualizations can allow us to think "with" space in ways that prosaic language cannot: "in the case of natural and artificial languages, internal connections exist among their fundamental components. In contrast, in the case of images, contiguity rules: they and their components are organized spatially into synchronous hierarchies or nested sets." "Unlike words," Gross writes, "images can undergo meaningful spatial transformations and

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[4] John W. CARROLL "Laws of Nature." *The Stanford Encyclopedia of Philosophy* [online] (Spring 2012 Edition), Edward N. Zalta (ed.), forthcoming URL <http://plato.stanford.edu/archives/spr2012/entries/laws-of-nature/>.

[5] David BIRDSELL – Leo GROARKE, "Outlines of a Theory of Visual Argument." *Argumentation and Advocacy*, vol. 43, 2007, no. 3–4, p. 106 (103–113).

[6] Alan G. GROSS, "Toward a Theory of Verbal–Visual Interaction: The Example of Lavoisier." *Rhetoric Society Quarterly*, vol. 39, 2009, no. 2, pp. 147–169.

manipulations, such as superimposition, projection, rotation, magnification, and animation."[7] A turn to the visual, non-verbal, and material is in the making for rhetoric of science. Propositionality becomes even more embedded in movable material models – as the (empirically discovered) structural protocols of molecules themselves (angles of attachment, sites of attachment, mobility and the like) are incorporated into designed materials, each piece and the way it relates to the whole becomes unquestionably true in the context of the model itself. Manipulatives – Watson and Crick's model, for example – combine the affordances of natural languages and visual ones; materials designed to have protocols relate both internally and spatially. Moreover, the protocols upon which material models depend have even less potential for the semantic slippage of verbal and visual arguments – they are, at least potentially, self-evident, obdurate objects in themselves.

The turn to the material is, of course, an ongoing trend in scholarship on both media and science, though scholars in interdisciplinary science studies rarely explicitly recognize the implications of their claims for media studies. Phenomenological accounts of how science thinks with and produces objects are perennial. Most notably, Hans-Jorg Rheinberger's *Towards a History of Epistemic Things* discusses how inquiry produces entire systems of materials –particularly lab-produced phenomena like cultures and protein replicators – to constitute a given field of knowledge,[8] and Davis Baird's *Thing Knowledge* focuses on the design of specialized instruments to manipulate the same.[9]

Historians who study knowledge-making in genetics are already examining media, and they are particularly interested in the inscription of images. Carol Keirns has documented geneticist Barbara McClintock's practices of "pictorial communication", and Keirns' description hints at the kind of inscription-reading expertise that Lorraine Daston and Peter Gallison turn in to a full-blown theory years later: "McClintock taught close colleagues to 'read' the patterns in her maize kernels, 'seeing' pigment and starch genes turning on and off."[10] Daston and Galison's 2007 book,

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[7] *Ibid.*, p. 148.

[8] Hans-Jorg RHEINBERGER, *Toward a History of Epistemic Things: Synthesizing Proteins in the Test Tube*. Stanford: Stanford University Press 1997.

[9] Davis BAIRD, *Thing Knowledge: A Philosophy of Scientific Instruments*. Berkeley: University of California Press 2004.

[10] Carol KEIRNS, "Seeing Patterns: Models, Visual Evidence and Pictorial Communication in the Work of Barbara McClintock." *Journal of the History of Biology,* vol. 32, 1999, no. 1, pp. 163–195.

Objectivity,[11] considers more cases like Keirns's, focusing on the materials – mostly machinery – and practices of image-rendering in the life sciences, and the way in which mediation has become a layer between the scientist and object of study. They argue that, though the media layer has been seen to remove the observer from the observed, such a "removal" is almost always more of a gesture – a social action, a convention of the community – than it is an actual separation. On the contrary – Gallison and Daston note that the specialization of inscription technologies makes it so that the expert scientist is even more tied to his or her product, as he or she must make sense of the image or rendering. Different types of inscription techniques and technology, different types of inscriptions themselves, and the resulting, extremely specialized inscription-reading practices become different types of objectivity.[12]

But the treatments of inscriptions I've described so far are all mediations based in visual representations or reproductions, not manipulative models. In their chapter of the same book entitled "Structural Objectivity", Daston and Galison note a scientific trend that paralleled the philosophical move to structuralism, and they say that "[scientists] who identified 'structures' as the core of objectivity understood a great variety of things under that rubric: logic, ordered sequences of sensations, some of mathematics, all of mathematics, syntax, entities that remain invariant under transformations".[13] Scientific structuralism, then, is at the basis of the experience and inscription of Ludwik Fleck's "system of uniformities"[14] – patterns that can become protocols in the recording, communicating, and manipulating of rules (maybe theories, laws), and concepts. Daston and Galison call the dependence on such structures a solution to "the specter of incommunicability in the sciences."[15] (It is no surprise, then, that a popular pre-med textbook is entitled *Organic Chemistry as a Second Language: Translating the Basic Concepts.*) Galison's essay "Ten Problems in History and Philosophy of Science" lists the structures and their inscription apparatus as "Problem number 3":

> *Technologies of Argumentation.* When the focus is on scientific practices (rather than discipline-specific scientific results *per se*), *what are the concepts, tools, and*

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[11] Lorraine DASTON – Peter GALLISON, *Objectivity*. Boston: Zone Books 2007.

[12] *Ibid.*

[13] *Ibid.*, p. 254.

[14] Ludwik FLECK, *Genesis and Development of a Scientific Fact*. Chicago: University of Chicago Press 1981.

[15] *Ibid.*

> *procedures needed at a given time to construct an acceptable scientific argument*? We already have some good examples of steps toward a history and philosophy of practices: *instrument making*, probability, objectivity, observation, *model building*, and collecting. We are beginning to know something of the nature of thought experiments—but there is clearly much more to learn. The same could be said for *scientific visualization*, where, by now, we have a large number of empirical case studies but a relatively impoverished analytic scheme for understanding how visualization practices work. So, cutting across subdisciplines and even disciplines, *what is the toolkit of argumentation and demonstration*—and what is its historical trajectory? [16]

Given Galison's name for the problem, a brand of scholarship that considers the material manipulatives with which scientists theorize must naturally go into the toolkit.

There are a few notable exceptions to the overall lack of scholarship on manipulative models and knowledge-making: the work of Eric Francoeur is one. In 1997, Francoeur called the "design and use" of physical molecular models a "forgotten tool [...] a constituitive yet overlooked element of chemical practices."[17] Francoeur's analysis of the differences between visual and spatial models and case-study historiography of model design is precisely the kind of work that my own inquiry strives to continue. Stephan Hartmann uses a case study in high-energy physics to define the term "model"; he determines that there are four types of model, and the "toy model" is one. Toy models and developmental models, he maintains, are "considerably useful in the process of theory construction", [18] i.e., toy models are a means of practicing scientific inductive reasoning. Even more recently, Adam Toon has used ethnographic sociology of science approaches to explore modeling. Toon watches scientists use models and interviews them about their attitudes towards them.[19] In two different articles explaining his findings, he uses a theory of make-believe from art studies to describe how scientists "imagine the models to be molecules, in much the same way that children

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[16] Peter GALISON, "Ten Problems in History and Philosophy of Science." *Isis*, vol. 99, 2008, no. 1, pp. 111–124 [emphasis mine].

[17] Eric FRANCOUER, "The Forgotten Tool: The Design and Use of Molecular Models." *Social Studies of Science*, vol. 27, 1997, no. 1, pp. 7–40.

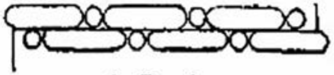
[18] Stephen HARTMANN, "Models as a Tool for Theory Construction: Some Strategies of Preliminary Physics." Accessed in PhilSci Archive, Reprint of a chapter from *Theories and Models in Scientific Processes*, Amsterdam: Rodopi 1995, pp. 49–67.

[19] Adam TOON, "The Ontology of Theoretical Modelling: Models as Make-believe." *Synthese*, vol. 172, 2010, no. 2, pp. 301–315.

imagine a doll to be a baby".[20] The "make-believe" step between the real and the representation resonates well with my own claim that models—and model pieces—are materially propositional—what Daston and Gallison call "entities that remain invariant under transformations",[21] stand-ins for *what is* that ostensibly behave just like *what is.*

More recently, scholars like Alan Rocke, Peter Ramberg, and the essays featured in a collection edited by Roman Frigg & Matthew Hunter have all treated representation in science and chemistry specifically. Rocke historicizes the drawings that enabled the beginning of modern organic chemistry,[22] and his story is where my own tracing begins. Ramberg takes up stereochemistry as an inscription-producing process.[23] The most pertinent recent scholarship, however, is Soraya de Chadarevian's edited collection that looks "back" on physical models as modeling practices move more and more to digital representations, which are arguably more detailed and less experientially embodied. Chadarevian's own chapter of the volume features the model as critical to the development of molecular biology as a discipline,[24] an argument that I will echo here. The epistemic impact of the "loss" of tanglible, embodied modeling remains to be seen; the arrangement and rearrangement of manipulative models is one well-established way that science reasons with materials.

From visual thinking to material thinking: a tracing



3. Benzine.

Figure 1: *Structure of Benzine as first visualized by Frederich August Kekulé.*
Source: *Friedrich August KEKULÉ, "Sur la constitution des substances aromatiques."* Bulletin de la Societe Chimique de Paris*, vol. 3, 1865, no. 2, pp. 98–110.*

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[20] Adam TOON, "Playing with Molecules." *Studies In History and Philosophy of Science Part A*, vol. 42, 2011, no. 4, p. 580.

[21] DASTON – GALISON, *Objectivity*, p. 254.

[22] Alan J. ROCKE, *Image and Reality: Kekulé, Kopp, and the Scientific Imagination*. Chicago: University of Chicago Press 2010.

[23] Peter RAMBERG, *Chemical Structure, Spatial Arrangement: The Early History of Stereochemistry, 1874–1914*. Aldershot – Burlington: Ashgate 2003.

[24] Soraya de CHADAREVIAN, "Models and the Making of Molecular Biology." *Models: the Third Dimension of Science*. Stanford: Stanford University Press 2004.

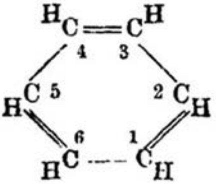

Figure 2: *Kekulé's ring structure as he proposes it at the end of the same paper.* Source: *Friedrich August KEKULÉ, "Sur la constitution des substances aromatiques."* Bulletin de la Societe Chimique de Paris*, vol. 3, 1865, no. 2, pp. 98–110.*

Most histories of organic chemistry and molecular biology include Frederich August Kekulé, and I will begin with him because he is credited with conceiving of the ubiquitous hexagonal and pentagonal ring structures at the heart of organic chemistry—the shapes that Watson and Crick made into metal plates to "stack" as the base center of their model. While Kekulé was working at the University of Ghent in Belgium, he conceived of the benzene ring in a now-famous dream about a snake swallowing its tail and published a paper postulating that the specific structures of organic compounds were likely as important as their formulae.[25] Kekulé's argument was the culmination of a general movement, caused by molecular theory, to include physics in chemistry—an obsession with discovering how the structure of molecules would predict their behaviors and properties. Kekulé and his contemporaries—most notably Josef Loschmidt and Alexander Crum Brown, who, John Wotiz, Ursula Klein, and Alan Rocke note, were devising graphic formulae four years before Kekulé published the same sort of work—necessarily invented a new notation to represent the structures. The big epistemic turn that Kekulé and his contemporaries made was to conceive of the angles of attachment as key to chemical behavior and interactivity (ultimately allowing for tetravalence and the entire field of organic and structural chemistry).[26] Wotiz maintains that Kekulé's visualizations worked to allow for a different kind of cognition than the (linear, mathematical) formulae that chemists had depended upon until then—the beginnings of a geometric thinking, a realization that what molecules did had much to do with their architecture

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[25] *Ibid.*

[26] ROCKE, *Image and Reality.*

in space.[27] Spatial reasoning was the basis of structural chemistry, and key to Linus Pauling's methodology (to be described later). Kekulé's work also hypothesized the variety and complexity of organic compounds to be discovered in the coming decades by Pauling and others.

Kekulé's student, Jacobus Henricus Van't Hoff, following Kekulé's assertion that chemicals' spatial arrangements were key to their chemical behavior, was one of the first to use toy-like models to do chemistry (Kekulé himself used "ball and stick models")[28] and the first to publish an argument for spatial modeling as a legitimate scientific methodology. According to Trienke M. Van der Spiek of the Booerhave Museum in the Netherlands, who has extensively historicized Van't Hoff's contributions to molecular modeling, Van't Hoff's argument, a pamphlet entitled *La chimie dans l'espace* (*Chemistry in space*), published in 1874, was before its time, representing "a major schism with the prevailing view of dimensionless molecules."[29] The epistemic context of the pamphlet is difficult to imagine with a contemporary mind; Van't Hoff had to argue against a way of thinking that didn't yet conceptualize objects as small as molecules actually occupying space in a way that was important to how they behaved physically or chemically. That step was a difficult enough paradigm shift for chemistry, but Van't Hoff also proposed new methodology. He began playing with toys – small paperboard triangles cut, color-coded, and folded into triangular solids to represent tetrahedral carbon atoms and their potential surrounding bonds. The models went through several iterations as Van't Hoff came to understand the asymmetrical shape of carbon and that shape's effects on its potential valences.[30] According to Van der Spiek, Van't Hoff's pamphlet described his models as "aids to visualization that made his hypothetical exegesis easier to understand and less strenuous to read"[31]—that is, they constituted a new form of technical communication, a spatial-material semiotic. Van der Spiek also points out that Van't Hoff's models are clearly designed to concentrate on potential attachments (and angles of attachments) around the carbon atoms in organic compounds, rather than being concerned with the location of the

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[27] John WOTIZ, *The Kekule Riddle: A Challenge for Chemists and Psychologists.* Vienna, IL: Glenview 1993.

[28] Trienke VAN DER SPIEKE, "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.

[29] *Ibid*., p. 160.

[30] Ursula KLEIN, *Experiments, Models, Paper Tools: Cultures of Organic Chemistry in the Nineteenth Century.* Stanford: Stanford University Press 2003.

[31] VAN DER SPIEKE, "Selling a Theory."

central atoms.[32] Van't Hoff, then, was concerned with a way to conceptualize the multitudes of possibilities for carbon-based arrangements – he wanted to imagine as-of-yet unobserved compounds. His models were for theorizing. His paperboard toys were hypothesis-makers for the most complicated chemical questions of the time.

That complexity was, of course, the bread and butter of an entire field of chemistry; for the good part of the next century, organic chemists devoted their careers, in part, to theorizing, finding, diagramming, and naming organic compounds. One product of that work was *The Ring Index: Ring systems used in organic chemistry*, published in 1940 by Austin Patterson and Leonard Capell, a 650-page listing of classes and individual molecular arrangements of known organic compounds, complete with instructions for subtle variations in names and notation – a field guide to organic chemistry's drawn representations. The "historical" section of the book's introduction notes that its compilation began in 1922, when a "Committee on the Preparation and Publication of a List of Ring Systems Used in Organic Chemistry" was formed from the Board of Editors of the Journal of the American Chemical Society. Writing was delayed by the Depression but finally completed in 1938, and the book claims to cover all classes of rings systematized through that year. [33]

Two things are particularly notable about *The Ring Index* for my purposes. The first is that it so clearly answers an exigence for the standardization of a symbolic language that uses known and empirically tested physical attributes of molecular structures to theorize about (and, later, design) the structures of unknown compounds. Secondly, the final and newest classes of ring system documented by the index (in 1938) are Class D1 and D2, simple spiro systems and complex spiro systems, respectively. The "spiro" class of system are the proto-helix—the structures that DNA will ultimately be discovered to have. Here the simple, two-dimensional drawings of the hydrocarbon/nitrogen shapes clearly begins to break down; the notation is cluttered by multiple numbers (to denote the number of atoms between "spiro atoms") and cross-hatched lines to denote bonds at certain angles (bond angles would, of course, be affected by this number). The basic pencil-and-paper notation fails to communicate the "structure" that is so key in structural chemistry and its deployment in molecular biology. At the end of

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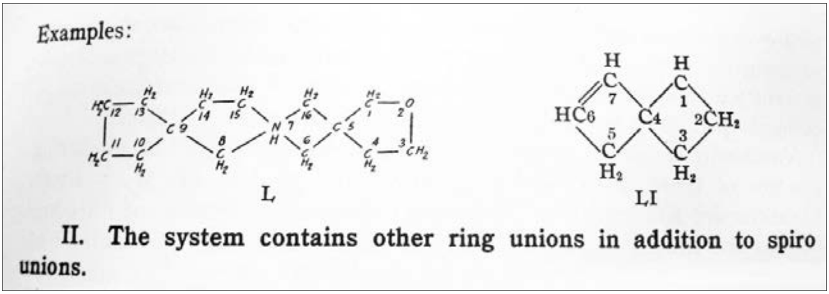
[32] *Ibid.*

[33] Austin M. PATTERSON – Leonard T. CAPELL, *The Ring Index: A List of Ring Systems Used in Organic Chemistry*, New York: Rheinhold 1940.

The Ring Index, the edited appendices offer a suggestion to chemists working with C3 class molecules and above: “In difficult cases it may be advisable to construct a spatial model so as to decide upon the most natural [plane formula and structure].”[34]



Examples:

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II. The system contains other ring unions in addition to spiro unions.

Figure 3: *Image from* The Ring Index: Ring Systems Used in Organic Chemistry *in the Spiro Class section. The notation required to denote the number and angle of attachments is outgrowing the capacity of the two-dimensional representation.* Source: *Austin M. PATTERSON – Leonard T. CAPELL,* The Ring Index: A List of Ring Systems Used in Organic Chemistry. *New York: Rheinhold 1940.*

The “Complex Spiro Systems” end the book, and the last line of the volume says of these systems: “Rule 24 [The rule pertaining to systems containing other ring unions in addition to spiro unions] has been marked ‘provisional’ because at some later time it may be thought desirable to give directions for numbering these systems ‘straight around,’ like the preceding classes. *No simple and certain way of doing this has yet been worked out*.”[35]

At the time of *The Ring Index*’s publication, Linus Pauling sat on the American Chemical Society’s Board of Editors; he is credited at the end of the index’s “General Introduction.”[36] It could easily have been Pauling who made the recommendation I’ve cited above, as spatial modeling was his preferred method of reasoning. He was known for his models, and many interviews and correspondences attest to the fact that models were his (theoretical) experiments – his way of thinking. During undergraduate school, Pauling was a machinist – a good one by his own lights, and it would seem

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[34] PATTERSON – CAPELL *Ring Index*, p. 607

[35] *Ibid*., p. 610 [emphasis mine].

[36] *Ibid*., p. 6

that his skill at space and shapes translated to a kind of material, structural intelligence. He was predisposed to think with models. In a 1964 interview with John Heilbron, Pauling exclaims, "[I have] always [made models], yes! [...] I still have the models [that he and the interviewer are discussing]. Here is the water molecule [showing the model]: the two electrons, here are the two electrons holding the hydrogen atom, these are the two K electrons. They don't need to be at that angle. I made these."[37] A paper Pauling published in the *Review of Scientific Instruments* in 1952, the year before Watson and Crick published the description of their structure, describes his models in detail. "Models representing atoms or groups of atoms built from hard wood to the scale 1 in.=1A are connected by a clamping device which maintains desired molecular configurations," says the abstract. Pauling goes on to say that "[t]hese accurate models have been used as substitutes for calculation in investigations of the probable configuration of the polypeptide chain in proteins. Analogous models constructed of rubber-like plastic to the scale 1 in. = 2A and connected by snap fasteners are designed for qualitative studies of protein structure."[38] Ultimately, Pauling's work with manipulatives won him recognition for a successful alpha model of the helical structure of amino acids – he proposed the structure that Watson and Crick's model was based on. When Watson and Crick proposed the complete double-helical model they had, in Watson's words, "beat Pauling at his own game."[39]

Pauling's "game", of course, was the combination of modeling and X-ray crystallography as the empirical measure to inform the physical protocols of his models. Pauling came up with the alpha helix model by using crystallography to determine the precise angles and architecture of the peptide bonds on a helical carbon chain and the structure of the residual atoms that would stack up against each other and cause the curve of the helix. According to Oregon State's special collections feature on Pauling, Pauling was ill and prescribed bed rest by his doctor when he sketched the molecules he was working with on a strip of paper and folded it along the same bond line, coming up with a helix. When he returned to the lab, he adjusted his model

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[37] Linus PAULING. "Oral History Transcript." In: *Niels Bohr Library and Archives* [online]. 1964. Available at <http://www.aip.org/history/ohilist/3448.html> [cit. 12. 10. 2012].

[38] Robert COREY – Linus PAULING, "Molecular Models of Amino Acids, Peptides, and Proteins." *Review of Scientific Instruments*, vol. 24, 1953, no. 8, pp. 621–627.

[39] James D. WATSON, *The Double Helix: A Personal Account of the Discovery of the Structure of DNA*. New York: Touchstone 1968, p. 48.

and drew up plans for a more robust, wooden version, which is now housed in Oregon State University's archives.[40]

Across a nation and an ocean, in England, James Watson and Francis Crick followed Pauling's lead and employed a methodology of model play, as well. Watson and Crick's story has been told by the men themselves and their close colleagues, and it has since been retold by historians, rhetoricians, and filmmakers; I do not mean to retell it again, here. But I do want to highlight the model itself – the metal plates and rods that the famous pair used as their primary, concrete argument – as a key character in the story. In some ways, the models Watson and Crick constructed were a way of responding to social constraints on their lab materials; they didn't have access to equipment or experimental, empirical data. Watson's account gives a scientist's rationale for his decision to use self-fashioned manipulatives: "I was soon taught that Pauling's result was a product of common sense, not the result of complicated mathematical reasoning [...] The key to Linus' success was his reliance on the simple laws of structural chemistry [...] the main working tools were a set of molecular models superficially resembling the toys of preschool children."[41] But Watson's description of his relationship to Wilkins' lab and Rosalind Franklin in particular imply the much more circumstantial reasons for his choice: he was a failure at growing myoglobin crystals, he was bad at math, X-ray analysis bored him, and, most importantly, even after he and Crick had made good progress on the model, they weren't able to produce the empirical evidence to "prove" their structure; "the crux of the matter was whether Rosy's new X-ray pictures would lend any support for a helical DNA structure [...] clues in constructing molecular models [... but Franklin's] determined mind had set upon a different course of action."[42]

If Watson and Crick were constrained by limited access to Franklin's empirical data, it can be argued that Franklin and Wilkins were equally constrained by their fixation upon it. And while Franklin (according to Watson) openly disdained Pauling's "game": "[t]he idea of using tinker-toy-like models to solve biological structures was clearly a last resort,"[43] Watson

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[40] All Documents and Materials, *Linus Pauling and The Nature of the Chemical Bond: A Documentary History*, Special Collections, Oregon State University [online]. n.d. Avaiable at <http://osulibrary.oregonstate.edu/specialcollections/coll/pauling/bond/materials/index.html> [cit. 6. 5. 2012].

[41] WATSON, *Double Helix*, p. 50

[42] *Ibid.*, p. 211.

[43] WATSON *Double Helix*, p. 69

and Crick were almost painfully dependent upon it, and at the mercy of the materials necessary to play. About John Kendrew's models—the first manipulatives that Watson and Crick have access to—Watson writes, "[they] would not be satisfactory [...] there existed no accurate representations of the groups of atoms unique to DNA [...] Rapid improvisation would be necessary since there was no time [...] to give a rush order for their construction."[44] Watson goes on to fashion his own stand-in parts out of copper wire, but he also relates the difficulty of theorizing without the proper materials and their inherent protocols: "Unlike the other constituents, [the inorganic ions] obeyed no simple-minded rules telling us the angles at which they would form their respective chemical bonds [...]we had to know the right DNA structure before the right models could be made."[45] In reference to conversations away from the models, Watson speaks of his own "inability to think in three dimensions [without the help of embodied interaction with the physical model],"[46] and the model's end game is fraught with waiting for new parts to come back from the machinist – time in which Watson, ironically, "decide[s] that no harm could come from spending a few days building backbone-out models."[47] In the end, even Maurice Wilkins seemed to understand that the "real" work was being done in the albeit artificial model – he urged Watson and Crick to delay their modeling in order to give his own lab time for the X-ray imaging and only hesitantly agreed to allow them to continue.

Francis Crick's memoir, which stretches into the uptake of the double helix into accepted theory and its subsequent growth into the field of molecular biology, discusses the importance of models as a means for theorizing and a way of knowing, as well. [48] He seems especially insistent that working in three dimensions is epistemically different than representation in two dimensions. He complains of having to remediate his work on to paper more than once. "Diagrams of models," he writes, "are often difficult to draw satisfactorily since, unless care is taken, they usually convey more than one intends."[49] The distinction between *thinking* with models and *communicating* with words – perhaps reducible, in rhetorical terms, to a difference in

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[44] *Ibid.*, p. 197.

[45] *Ibid.*, p. 195.

[46] *Ibid.*, p. 155.

[47] *Ibid.*, p. 158.

[48] Francis CRICK, *What Mad Pursuit: A Personal View of Scientific Discovery*. New York: Basic Books 1990.

[49] *Ibid.*, p. 46.

audience – is a fascinating one. Crick's commentary echoes the concepts that Francoeur describes in his work on particle physics.

In another compelling section of Crick's book, he discusses at length the theoretical "mistakes" that he made when working to develop many of his theories, mistakes that he was able to understand better at the time of writing his memoir, as theoretical and empirical knowledge continued to be built upon the helix as a basic structure for the gene (specifically the role of RNA in replicating genetic information). One of these bears mentioning here because it speaks to the way he thought about the models. He writes:

> It is clear that I thought of the RNA in the cytoplasm [...] as a "template," that is, having a rather rigid structure comparable to the double helix of DNA but probably having one single chain. It was only later that I realized that this was too restrictive an idea, and that "tape" might be nearer to the truth [...] I eventually realized that RNA need not be rigid, but could be flexible, except for the part that coded the next amino acid to be incorporated. Another consequence of this idea was that the growing protein chain did not have to stay on the template but could start to fold itself up as the sequence proceeded, as indeed had been suggested earlier.[50]

The complex process of protein folding and its tremendous impact on the action of proteins has become, of course, the next big problem for material manipulative reasoning to solve in molecular biology and genetics.

Manipulative Models in the Public Imagination: an archive of advertisements and images

At the same time that Watson, Crick, Franklin, Wilkins et al. were doing their work in labs largely inaccessible to the layman, models as ways of seeing and knowing about the sub-visible world were already common to the public imagination, thanks to Kekulé's epistemic legacy. An illustrated *Popular Mechanics* article from 1928 pictures Henry D. Hubbard, then secretary of the U.S. Bureau of Standards, with models designed to depict organic compounds. "One of his sets of models," the magazine tells its lay audience, "depict[s] the formation of carbon nuclei, carbon atoms, and diamonds [...] Strength and hardness are due to the arrangement of the atoms, and clarity to the 'space patterns' which their particular arrangement provides."[51]

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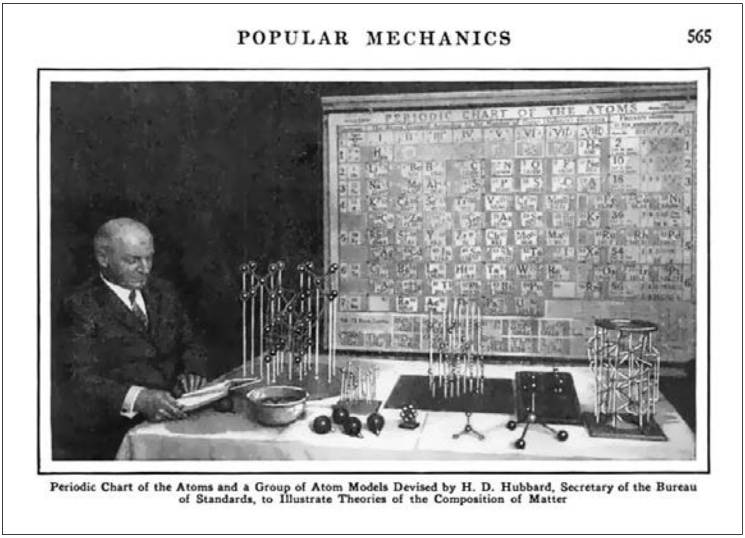
[50] CRICK, *What Mad Pursuit,* p. 110.

[51] *Ibid,* p. 560.

Hubbard worked for the Bureau of Standards, a position that resonates with Pauling's interest in the Committee for Chemical Nomenclature and the standardizing force of the Ring Index – scientists involved with modeling were acutely aware of the need for a consistent material language.[52]



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Periodic Chart of the Atoms and a Group of Atom Models Devised by H. D. Hubbard, Secretary of the Bureau of Standards, to Illustrate Theories of the Composition of Matter

Figure 4: *Image from an article in* Popular Mechanics *from 1928, depicting Henry Hubbard and wooden models of organic compounds.*
Source: Popular Mechanics*, Volume 50.4, October 1928.*

Later, in the 1940s, models like Hubbard's were ultimately marketed to parents and school systems as pedagogical tools, and the propositional materials of manipulative models became their own kind of publicly accepted facts. Probably the most influential of these models was the Fischer-Taylor-Hirschfelder Atom Model Kit. It was used in high school chemistry courses.

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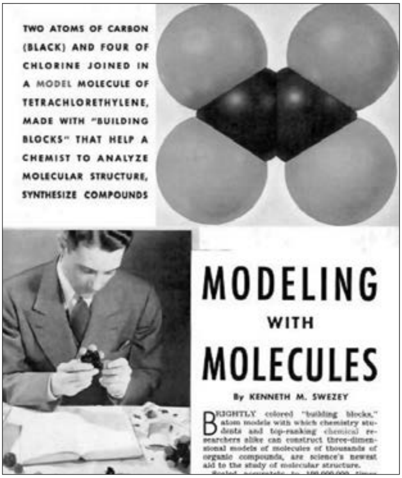
[52] For a recent treatment of the intersection of the specific problematics of modeling and issues of standardization, see Adrian MACKENZIE – Claire WATERTON – Rebecca ELLIS – Emma FROW – Ruth McNALLY – Lawrence BUSCH – Brian WYNNE, "Classifying, Constructing, and Identifying Life: Standards as Transformations of 'The Biological'." *Science, Technology & Human Values*, 2013.

Figure 5: A basic Fischer atomic modeling kit from the 1940s.
Source: "1940s Vintage Wooden Atomic Model Kit." Factory 20 [online]. n.d. Available at <http://www.factory20.com/objects/1940s-vintage-wooden-atomic-model-kit/> [cit. 6. 5. 2012].



TWO ATOMS OF CARBON (BLACK) AND FOUR OF CHLORINE JOINED IN A MODEL MOLECULE OF TETRACHLORETHYLENE, MADE WITH "BUILDING BLOCKS" THAT HELP A CHEMIST TO ANALYZE MOLECULAR STRUCTURE, SYNTHESIZE COMPOUNDS

MODELING
WITH
MOLECULES

By KENNETH M. SWEZEY

BRIGHTLY colored "building blocks," atom models with which chemistry students and top-ranking chemical researchers alike can construct three-dimensional models of molecules of thousands of organic compounds, are science's newest aid to the study of molecular structure.

Figure 6: *The same Fischer kit featured in* Popular Science *in 1942.*
Source: Popular Science*, June 1942.*

The most basic kit included five isotopes of nitrogen and five isotopes of carbon, three of sulfur, two of oxygen, and one piece-type each to represent the elements bromine, iodine, and chlorine. Models using the set look like nubby caterpillars with dark blue and black middle bodies – the dark blue being nitrogen, black being carbon. Where the oxygen, hydrogen, bromine, iodine and chlorine pieces are semi-circle bubbles that attach to the flat side of carbon and nitrogen, C and N are triangular wedges that work together to make hexagonal and pentagonal centers – echoes of Van't Hoff's triangular arrangements of carbon. These same models are featured in a story in *Popular Science* in 1942 that explains to its readers exactly how scientists think with models. In it, models are hailed as science's "newest aid to the study of molecular structure." The article, which is a history of modeling practices, even touches upon my own question of the fluidity of scientific knowledge production and the concretized, material propositionality of the standardized wooden models. "Until a few years ago," the journalist writes, "knowledge of the architecture of organic compounds was not sufficiently complete to allow for accurate representation," and models, he claims, were "crude" and vague.[53] Later, the article describes the models' relationship to the basic assumptions of structural chemistry quite well; "Investigation of some 500 compounds by electron diffraction revealed that the different forms of building blocks required to make them were surprisingly few. In fact, most organic compounds could be represented accurately by molecule models built up from less than two dozen kinds and shapes of atom models."[54] Complexity is made up of meaningful combinations and recombinations of very simple elements. The world is a toy sculpture made of structural protocol. With good representational tools for arrangement, the article seems to promise, we can inductively find its structure and even invent new structures that play according to the existing world's rules.

Popular magazines provide evidence that modeling as a pedagogical practice was still flourishing into the 1960s and 70s. In 1963, *LIFE* magazine devoted a whole page and a half to advertising for at-home science kits, including a "Chemcraft Master Deluxe Lab" that boasted an "atomic model kit," along with a centrifuge, molecular balance, and spectroscope.[55] In 1971, Great Britain's *New Scientist* reviewed A. F. Wells's *Models in structural inorganic chemistry (with model building set)*, a text that describes the practice of

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[53] *Ibid*, p. 42.

[54] *Ibid*, p. 42.

[55] *LIFE* magazine, November 22, 1963, p. 11.

modeling in structural chemistry. According to reviewer Jeffrey Cox, Wells "elaborates the theme that the builder of a model gains a deep insight into the structure it represents."[56] Cox applauds the publisher on its "enterprise [… in including a model in the text] here is a plentiful supply in a single kit for building ball-and-stick, pack of spheres, and joining-of-polyhedra models. Each type of model emphasizes a particular aspect of structure: spatial relationships, steric requirements of ions, and the coordination of atoms. Both teacher and learner can profit from this multiplicity of emphasis."[57] Standardized modeling tools for structural chemistry, then, were taken for granted as thinking and learning tools by the 1970s.

Conclusion: A snapshot in the present

Modeling as efficacious pedagogy is still being studied; I'll briefly describe two examples from the *Journal of Research in Science Teaching*, here. "The use of three-dimensional visualization as a moderator in the higher cognitive learning of concepts in college level chemistry," by Lawerence H. Talley, argues for the use of material models in student labs, not just for teacher demonstration, because modeling is an enhancement of visualization skills essential to higher-level chemistry. [58] In "Effect of Bead and Illustrations Models on High School Students' Achievement in Molecular Genetics", Yosi Rotbain, Gili Marbach-Ad, and Ruth Stavy report the results of an empirical study of pedagogical practices in high school genetics classes and conclude that "it is advisable to use a three-dimensional model, such as the bead model" [59] to engage students in conceptualizing genetic action at the molecular level.

And at the level of knowledge-making in university and private labs, the tools used to design and interact with models are changing and evolving, as well—spatial and material modeling is a living methodology in molecular biology and related fields. The *Foldit*[60] project out of the University of

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[56] Jeffrey COX, Book Review, *New Scientist*, July15, 1971, p. 159.

[57] *Ibid.*

[58] Lawrence H. TALLEY, "The Use of Three-dimensional Visualization as a Moderator in the Higher Cognitive Learning of Concepts in College Level Chemistry." *Journal of Research in Science Teaching*, vol. 10*, 2006,* no. 3, pp. 263–269.

[59] Yosi ROTBAIN – Gili MARBACH-AD – Ruth STAVY, "Effect of Bead and Illustrations Models on High School Students' Achievement in Molecular Genetics." *Journal of Research in Science Teaching*, vol. 43, 2006, no. 5, p. 525 (500–529).

[60] *Foldit*, University of Washington [online]. Available at: <http://fold.it/portal/> [cit 12. 10. 2012].

Washington, for example, employs designers from the UW Center for Game Science to maintain a computer game whose object is protein folding to predict and produce data about the structures of heretofore unknown organic compounds.

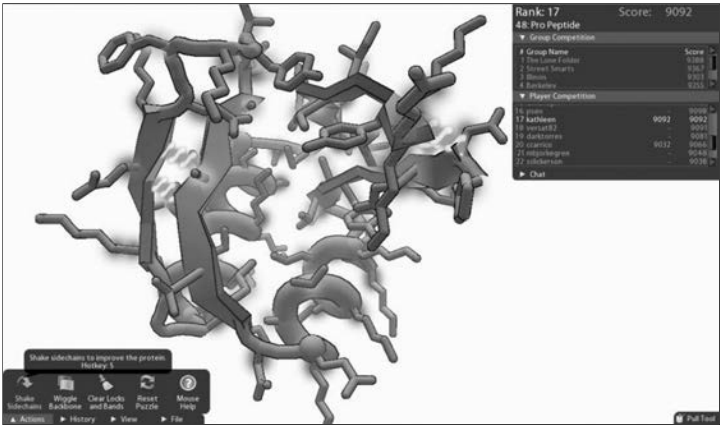

Figure 6: *Foldit's puzzle interface*
Source: Foldit*, University of Washington [online]. Available at <http://fold.it/portal/> [cit 12. 10. 2012].*

Foldit's interface is a three dimensional on-screen manipulative, but its genre is a multi-player online game; the protocols of the game turn all users—anyone who signs up for an account—into modelers. The game produces data to answer real scientific exigencies: "Figuring out which of the many, many possible structures is the best one is regarded as one of the hardest problems in biology today and current methods take a lot of money and time, even for computers. *Foldit* attempts to predict the structures of proteins by taking advantage of humans' puzzle-solving intuitions and having people play competitively to fold the best proteins. Players can design brand new proteins that could help prevent or treat important diseases" (*Foldit*, About). The website goes on to detail how protein folding and protein design could contribute to knowledge-building about therapies for HIV/AIDS, Cancer, and Alzheimer's Disease. *Foldit* clearly takes the Tinker-Toy ethos to a new and fascinating level – one Linus Pauling would approve of, I think. *Foldit* and other crowd-sourced approaches to science take Watson, Pauling, and Franklin's idea of model-manipulation as "playing with toys" or "beating [another scientist] at his own game" out of the realm of analogy. The move implies new questions for study of philosophical toys: how does gamification change the knowledge-making process by allowing for the manipulation of "big data"? What new roles does the object-as-model take on when it becomes a multi-player game? And what are the implications of the remediation of the three-dimensional model through digital tools rather than hands-on materials like metal, plastic and wood?