Paper Chemistry: François Dagognet and the Chemical Graph

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Abstract: In two books published in 1969 and 1973, the philosopher François Dagognet articulated a sharp contrast between the verbal and the visual in the history of chemical representation. Ursula Klein took up Dagognet's argument as both inspiration and foil in her account of Berzelian formulas as productive "paper tools." Building on Klein's work, I show how Dagognet portrayed chemical names and formulas not just as representations and paper tools, but as material abstractions that were objects of inquiry in themselves. Dagognet associated this way of doing chemistry with chemists' use of computers, citing the work of the physical organic chemist Jacques-Émile Dubois. However, I show that chemical editors and mathematicians had begun to treat chemical names and formulas in this way long before anyone used computers for such studies. Indeed, some of the techniques of graph theory central to the application of computers to chemistry in the mid-twentieth century were themselves in part derived half a century earlier from the application of chemical formulas to mathematical reasoning.

In 1890, August Kekulé took credit for introducing a "living, spatial conception" of atomic arrangements into structure theory. Without the aid of his architect's imagination, Kekulé asserted, structure theory "would have become merely a 'paper chemistry.'"[1] In making this claim, Kekulé invoked a critique that chemists had lobbed back and forth for decades: that of playing "games with formulas," retreating from chemical theories and empirical evidence into a formalist study of written representations. The "living, spatial conception" of chemical substances and phenomena, as expressed in visually suggestive diagrams, three-dimensional physical models, and computer graphics, has attracted considerable attention

[1] Richard Anschütz, ed., *August Kekulé*, vol. 2 (Berlin: Verlag Chemie, 1929), 944, quoted in Alan Rocke, "Vinegar and Oil: Materials and Representation in Organic Chemistry," in *Objects of Chemical Inquiry*, ed. Ursula Klein and Carsten Reinhardt (Sagamore Beach, MA: Science History, 2014), 47–60, on 56.

from historians and philosophers of chemistry.[2] "Paper chemistry" has not. Yet since the mid-twentieth century, chemists have come to depend upon methods, especially computer-based methods, grounded in just the sort of manipulations that Kekulé maligned.[3]

Whenever chemists search for compounds containing a particular molecular substructure, ask whether a chemical is subject to patent protection, generate lists of compounds to test out as potential new drugs, or carry out other tasks that involve dealing with many chemicals at once, they do so by means of *chemical graphs*.[4] These chemical graphs are structural formulas reinterpreted as abstract collections of associations (bonds) between units (atoms). The graphs are not merely representations of chemical substances, but conceptual entities with their own formal properties, which may be expressed using various notations accommodated to direct interpretation and/or machine processing. Chemical graphs are abstractions, but they are also material, in two senses: they are taken as epistemically relevant in themselves, and the forms in which chemists address them – structural formulas, systematic names, alphanumeric ciphers, topological matrices – have a

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[2] Alan J. Rocke, *Image and Reality: Kekulé, Kopp, and the Scientific Imagination* (Chicago: University of Chicago Press, 2010); Pierre Laszlo, *La parole des choses, ou, le langage de la chimie* (Paris: Hermann, 1993); Stephen J. Weininger, "Contemplating the Finger: Visuality and the Semiotics of Chemistry," *Hyle* 4 (1998): 3–27; Natasha Myers, *Rendering Life Molecular: Models, Modelers, and Excitable Matter* (Durham: Duke University Press, 2015); Jeremiah James, "Modeling the Scale of Atoms and Bonds: The Origins of Space-filling Parameters," in Klein and Reinhardt, *Objects of Chemical Inquiry*, 281–320; Christoph Meinel, "Molecules and Croquet Balls," in *Models: The Third Dimension of Science*, ed. Soraya de Chadarevian and Nick Hopwood (Stanford: Stanford University Press, 2004), 242–75; Soraya de Chadarevian, "Models and the Making of Molecular Biology," in Chadarevian and Hopwood, *Models*, 339–68; Eric Francoeur and Jérôme Segal, "From Model Kits to Interactive Computer Graphics," in Chadarevian and Hopwood, *Models*, 402–29.

[3] A related but distinct usage of "paper chemistry" refers to "thought experiments" running inverse to laboratory experiments, which chemists use to plan and interpret their material manipulations; Jeffrey I. Seeman, "On the Relationship between Classical Structure Determination and Total Synthesis," forthcoming in *Israel Journal of Chemistry* 57 (2017).

[4] Peter Willett, "Chemoinformatics: A History," *Wiley Interdisciplinary Reviews: Computational Molecular Science* 1 (2011): 46–56, on 49–50. On the history of chemical applications of graph theory, see also Alexandru T. Balaban, "Chemical Graph Theory and the Sherlock Holmes Principle," *Hyle* 19 (2013): 107–34. For an overview of chemical graphs and their use in present-day chemistry, see David Wild, *Introducing Cheminformatics,* ed. 2.0 (Published electronically: David Wild, 2012–2013).

concreteness that allows certain manipulations and resists others. If, as Ursula Klein has shown, chemists employ formulas as "tools on paper" for conducting theoretical and experimental investigations, then chemical graphs are *objects* of investigation, on paper, screens, and disks.

Building on Klein's analysis of chemical representations as paper tools, this essay outlines a history of how chemical representations became material abstractions of this sort.[5] Like Klein, I will delve into the work of François Dagognet, a distinguished philosopher who presented an eccentric but penetrating semiotic history of chemistry in two books published in 1969 and 1973. Klein draws on Dagognet's account of verbal and visual notation as both inspiration and foil for her argument. Contrary to Dagognet's dismissal of Berzelian formulas as mere verbal representations, Klein shows that chemists of the 1820s, 1830s, and 1840s used these formulas as graphically suggestive tools for investigating chemical constitution and reactions, classifying chemical compounds, filling in gaps between laboratory instruments, and, ultimately, constructing the experimental culture of organic chemistry. Yet Dagognet's work on chemical semiotics went beyond the distinction between names and images. He argued that the emergence of the computer-based chemistry of the future would entail a retreat from visuality into a kind of

[5] Ursula Klein, *Experiments, Models, Paper Tools: Cultures of Organic Chemistry in the Nineteenth Century* (Stanford: Stanford University Press, 2003). By referring to chemical graphs as "material abstractions," I do not mean to suggest that the abstract idea of a chemical graph is somehow material. Rather, I wish to draw attention, first, to the concrete (material) renderings of formal properties of chemical graphs, which differ according to the modality and medium in which they are rendered. Second, I wish to capture how such concrete renderings of formal properties become salient (material) when, abstracting from their function as representations of chemical compounds, these renderings and the formal properties they embody are addressed as objects of inquiry. Such "cheminformatic" activities constitute a significant part of recent chemistry; a sympathetic reading of Dagognet helps bring them into focus. I thank Michael Barany for suggesting the term "material abstractions" and an anonymous reviewer for pointing out its drawbacks. On the reshaping of abstractions through "implementation," that is, accommodation to the materiality of digital computing, see Stephanie Dick, "Of Models and Machines: Implementing Bounded Rationality," *Isis* 106 (2015): 623–34.

representation more tractable to manipulation by machine.[6] By Dagognet's lights, this new approach to chemistry was nothing less than an "authentic 'Copernican Revolution,'" in which "the material science of chemistry will be reduced, in part, to a third-order science of organization."[7]

In his preoccupation with representation, Dagognet did not have much to say about the material science of chemistry in the first place. Bernadette Bensaude-Vincent has suggested that this is one reason that his work has received relatively little attention from historians.[8] Yet Dagognet's interest in signs rather than substances makes his work a good point of departure for exploring a different sort of materiality: the materiality of inscriptions.[9] Writing about the processes of sequencing and analysis that have come to dominate contemporary molecular biology, the historian Hallam Stevens has argued that "materiality is never fully erased, but rather, the material of the organism and its elements is replaced with other sorts of material: computer screens, electrons, flash memory, and so on."[10] The same goes for chemical graphs. Moreover, as historians have shown in the cases of geology and government, for example, the application of computers to chemical

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[6] This is broadly parallel to the distinction that Peter Galison draws in his analysis of cultures of representation in particle physics, in which he contrasts the "homomorphic" images rendered by bubble chamber detectors to the "homologous" logic of particle counters; Peter Galison, *Image and Logic: A Material Culture of Microphysics* (Chicago: University of Chicago Press, 1997), 19–31.

[7] François Dagognet, *Écriture et iconographie* (Paris, Vrin, 1973), 124; François Dagognet, *Tableaux et langages de la chimie: Essai sur la représentation* (Seyssel: Champ Vallon, 2002 [1969]), 156 (cited hereafter as *ÉI and TL,* respectively). All translations are mine except where otherwise noted.

[8] Bernadette Bensaude-Vincent, "Dagognet et la chimie," in *François Dagognet épistémologue*, ed. Bernadette Bensaude-Vincent, Jean-François Braunstein, and Jean Gayon (Paris: Éditions Matériologiques, forthcoming 2018).

[9] Bruno Latour, "Visualisation and Cognition: Drawing Things Together," in *Knowledge and Society: Studies in the Sociology of Culture Past and Present*, ed. Henrika Kuklick and Elizabeth Long, vol. 6 (Jai Press, 1986), 1–40 (discussion of Dagognet on 13–14).

[10] Hallam Stevens, *Life out of Sequence: A Data-Driven History of Bioinformatics* (Chicago: University of Chicago Press, 2013), 8.

representation was enabled by and perpetuated existing forms of chemical representation.[11] Computers did not transform chemical formulas into material abstractions; rather, computers could be applied to the manipulation of chemical formulas because chemical formulas had already been made into material abstractions.

Dagognet identifies chemical information as the site of the epistemic crisis that catalyzed the transformation of chemistry into a "science of organization." Scholars of the history of information have argued convincingly that the information repositories they study are not abstract records of knowledge, but "paper technologies," "paper machines," "paper knowledge," and "paper tools," epistemically generative material artifacts.[12] Such *documentary* paper tools are different from the *investigative* paper tools that Klein discusses. Documentary paper tools aim to address the excess of trustworthy information – the persistent problem that there is too much to know.[13] Investigative paper tools address inconsistency and uncertainty.[14] Documentary paper tools freeze names, classifications, and data into a fixed form and order, facilitating storage and access to knowledge, and generating new knowledge about and through many objects.[15] Investigative paper tools

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[11] David Sepkoski, "Towards 'A Natural History of Data': Evolving Practices and Epistemologies of Data in Paleontology, 1800–2000," *Journal of the History of Biology* 46 (2013): 401–44; Jon Agar, *The Government Machine: A Revolutionary History of the Computer* (Cambridge, MA: MIT Press, 2003).

[12] Lisa Gitelman, *Paper Knowledge: Toward a Media History of Documents* (Durham: Duke University Press, 2014); Markus Krajewski, *Paper Machines: About Cards & Catalogs, 1548-1929*, trans. Peter Krapp (Cambridge, MA: MIT Press, 2011); James Delbourgo and Staffan Müller-Wille, eds., "Listmania," Focus section of *Isis* 103 (2012), 710–52; Robert E. Kohler and Kathryn M. Olesko, "Introduction: Clio Meets Science," *Osiris* 27 (2012): 1–16, on 2; Lorraine Daston, ed., *Science in the Archives* (Chicago: University of Chicago Press, 2017); Elena Aronova, Christine von Oertzen, and David Sepkoski, eds., "Data Histories," *Osiris* 32 (2017); Seth Rockman, ed., "The Paper Technologies of Capitalism," Forum section of *Technology and Culture* 58 (2017): 487–569.

[13] Ann Blair, *Too Much to Know: Managing Scholarly Information before the Modern Age* (New Haven: Yale University Press, 2010).

[14] See Michael Gordin's essay in this issue.

[15] Geoffrey C. Bowker, *Memory Practices in the Sciences* (Cambridge, MA: MIT Press, 2005).

render experimental results, theories, and classifications malleable in order to generate new scientific insights about and through individual objects.[16] The right tools for the jobs of documentation and investigation are typically quite different: documentary paper tools are things like reference books, card files, and electronic databases, along with their indexes, classification codes, organisational schemata, and metadata, whereas investigative paper tools, in Klein's sense, are things like Berzelian formulas, Feynman diagrams, and circuit diagrams.[17]

In structural organic chemistry at the end of the nineteenth century, documentary paper tools and investigative paper tools became closely entwined. A group of chemists stabilised structural formulas as systematic chemical names, intended to function as building blocks for documentary paper tools. Victorian mathematicians Arthur Cayley and James Joseph Sylvester took structural formulas as a starting point for developing objects of mathematical inquiry. To refer to these objects, Sylvester coined the term "chemical graph," a category that he later generalised as "graph." The mathematical study of such graphs – "graph theory" – subsequently took on an important role in the development of applied mathematics and computing. Chemists and mathematicians engaged these material abstractions in different ways and for different purposes. However, their shared genealogy and shared form enabled them to come together in computer-based chemical information systems of the 1960s.

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[16] Klein, *Experiments, Models, Paper Tools*; David Kaiser, *Drawing Theories Apart: The Dispersion of Feynman Diagrams in Postwar Physics* (Chicago: University of Chicago Press, 2005); Andrew Warwick, *Masters of Theory: Cambridge and the Rise of Mathematical Physics* (Chicago: University of Chicago Press, 2003).

[17] On the transformation of investigative paper tools into documentary paper tools and back again, see the discussion of "writing up" and "reading down" in Michael J. Barany and Donald MacKenzie, "Chalk: Materials and Concepts in Mathematics Research," in *Representation in Scientific Practice Revisited*, ed. Catelijne Coopmans et al. (Cambridge, MA: MIT Press, 2014), 107-29.

Taking Klein's use of Dagognet as a starting point, the first section of this essay follows the thread of an account of paper tools, material abstractions, and chemical documentation that winds through Dagognet's writings on the semiotic history of chemistry. The second section briefly addresses the DARC system of the physical organic chemist Jacques-Émile Dubois, which Dagognet labeled a "Copernican revolution" in computer-based chemistry. Dubois used chemical graphs as a means of simultaneously solving problems of documentation and interpretation of physical analytical data. The third section of this essay recounts the development of systematic chemical nomenclature, methods for counting isomers, and chemical graphs. In different ways, the architects of each took structural formulas as objects of inquiry, helping to establish the foundations of graph theory and its application to chemistry. The conclusion sums up Dagognet's account of "scriptural chemistry" and a few promising lines of historical inquiry that it suggests.

"A chemistry which turns itself into a science of writing"

In her account of Berzelian formulas as investigative paper tools, Ursula Klein draws upon and critiques François Dagognet's analysis of the virtues of visual chemical representation in his books *Tableaux et langage de la chimie* (1969) and *Écriture et iconographie* (1973). Dagognet dismissed Berzelian formulas as chemical "stenography" – mere transcriptions of spoken names. This dismissal, however, was an intermediate stage in his broader argument about transformations in the practice of chemistry. Dagognet contended that the goals of organic chemistry and its objects of inquiry changed between the late nineteenth and the mid-twentieth century. According to him, chemistry was no longer primarily focused on investigations of individual substances. It had become a "science of organization" addressing written or digital traces. This is an intricate and suggestive argument with some

apparent historical shortcomings. For the most part, I do not aim to evaluate it (still less to affirm it), but rather to explicate this argument and show how it can be put to use as a guide for developing a novel perspective on the history of chemistry.

Before delving into Dagognet's argument, it is worth noting that the idea of a chemistry that took formulas to be material abstractions was by no means outlandish to chemists in the nineteenth century – just the idea that such chemistry could possibly be worthwhile. Auguste Laurent accused Jacob Berzelius of making chemistry a "science of bodies that do not exist" in his use of dualistic formulas.[18] Justus Liebig accused Laurent of "arbitrary play with ideas and formulas to which he attributes a significance they do not have."[19] Hermann Kolbe accused Charles Gerhardt, Jean-Baptiste Dumas, and August Kekulé of "*Formelspiel*," playing "formula games" (in his later years, Kolbe extended the critique to contemporary chemistry in general).[20] Kekulé criticised "the mischief of those who make a game of constitutional formulas."[21] August Wilhelm Hofmann once accused *himself* of playing a formula game, a self-critique aimed at qualifying his claims about the constitution of quinine and other alkaloids.[22] Though such critiques have sometimes been chalked up to skepticism of atomism, structure theory, visual thinking, or theoretical

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[18] Auguste Laurent, *Méthode de chimie* (Paris: Mallet-Bachelier, 1854), x, quoted in Bernadette Bensaude-Vincent and Jonathan Simon, *Chemistry: The Impure Science*, 2nd ed. (London: Imperial College Press, 2012), 108.

[19] Quoted in John Hedley Brooke, "Laurent, Gerhardt, and the Philosophy of Chemistry," *Historical Studies in the Physical Sciences* 6 (1975): 405–29, on 420.

[20] H. Kolbe, "Ueber den natürlichen Zusammenhang der organischen mit den unorganischen Verbindungen," *Annalen der Chemie und Pharmacie* 113 (1860): 293–332, on 294. See Alan J. Rocke, *The Quiet Revolution: Hermann Kolbe and the Science of Organic Chemistry* (Berkeley: University of California Press, 1993), 150, 199.

[21] Kekulé to L. Meyer, 23 October 1860, in Anschütz, *Kekulé*, vol. 1, 205, quoted in Rocke, *Quiet Revolution*, 220.

[22] August Wilhelm Hofmann, "Beiträge zur Kenntniss der flüchtigen organischen Basen," *Annalen der Chemie und Pharmacie* 79 (1851): 11–39, on 31.

speculation, Alan Rocke and others have shown that chemists made use of all of these modes of reasoning while accusing their rivals of playing formula games. Kekulé at first rejected the graphical formulas of Couper and Crum Brown because they were not visualisable *enough*; Kolbe took issue with "formula games" for their *detachment* from chemical theory.[23] The chemist Benjamin Brodie Jr. leveled the critique at colleagues for their use of graphical formulas, and they threw it back at him regarding his algebraic "calculus of chemical operations."[24] Nobody defended the chemistry of formula games; like "spirit of system" among Enlightenment *philosophes* or "pseudoscience" in mid-twentieth century America, it was strictly a term of abuse.[25] Klein noted that although paper tools "embody intellectual assumptions, they are no longer epistemically relevant in themselves."[26] Nineteenth-century references to formula games were accusations of attributing epistemic relevance to inscriptions in themselves rather than to the phenomena and principles that they modeled.

Dagognet took an interest in chemical formulas for what he thought they could offer philosophy. A physician and philosopher who trained with Georges Canguilhem, Dagognet began his career writing about medicine and the life sciences. His subsequent work spanned a wide range of subjects in the philosophy of science, technology, aesthetics, and morals.[27] He took up chemistry, he wrote, as an intellectually productive and historically significant subject within the general philosophical study of representation. Drawing on J.

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[23] Rocke, "Vinegar and Oil," 56–57.

[24] Stephen T. Irish, "Brodie's Calculus and Chemical Classification," *Ambix* 60 (2013): 234–54.

[25] Jessica Riskin, *Science in the Age of Sensibility: The Sentimental Empiricists of the French Enlightment* (Chicago: University of Chicago Press, 2002); Michael D. Gordin, *The Pseudoscience Wars: Immanuel Velikovsky and the Birth of the Modern Fringe* (Chicago: University of Chicago Press, 2012).

[26] Klein, *Experiments, Models, Paper Tools*, 3.

[27] Gérard Chazal and Christian Salomon, *François Dagognet: médecin et philosophe* (Paris: Harmattan, 2005).

R. Partington's four-volume *History of Chemistry* for subject matter, he aimed to show historians and philosophers of science that "certain intellectual notions come out refreshed from a light chemical bath."[28] Dagognet took the history of science as an inquiry into intellectual clashes and ruptures, seismic shifts in epistemology, ontology, and methodology.[29] He also emphasised that scientists tended to reinterpret these ruptures in a way that both resolved them in the present and effaced them from the past. Furthermore, Dagognet was committed to a philosophical account that supported a history of continuous progress in science and technology.[30] He therefore endeavored to recover moments of rupture without portraying them as unbridgeable breaks: a dialectical history of progress across discontinuity.[31]

In *Tableaux et langages de la chimie,* Dagognet took up the history of chemical representation from Antoine Lavoisier through Dagognet's mid-twentieth-century present day. He distinguished three modes of chemical representation: the verbal, the visual, and the tableau. Dagognet's account of verbal representation followed what he called "voco-structural" correspondence: the ideal of bringing chemical objects, names, and ideas into a fixed and transparent relation. Locating the origin of this project in Lavoisier's application of Condillac's conception of science as well-made language, Dagognet traced chemists' continuing efforts to "make reality translate itself, reflect itself in a transparent method of naming."[32] Dagognet presented pictorial chemistry as arising when verbal representation

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[28] *TL*, 5.

[29] *ÉI*, 123.

[30] Daniel Parrochia, "French Philosophy of Technology," in *French Studies in the Philosophy of Science*, ed. Anastasios Brenner and Jean Gayon (Dordrecht: Springer, 2009), 51–70, on 64.

[31] *TL*, 86.

[32] On nomenclature in eighteenth-century chemistry, see Wolfgang Lefèvre's essay in this issue.

ran into epistemic roadblocks, taking the place of chemical names "when the word collapses." The tableau – the French, like the English, denotes both "table" and "picture" – brought together elements of the verbal and visual, aiming not just at "the translation of one substance, but the expression and the image of all." The tableau was a "chemical family photo," a "map of the ensemble of material continents," depicting "the totality of substances, along with the properties of each of them and the multiplicity of relationships that ties it to the others."[33] Dagognet's signal example of the tableau was the periodic table, but he equally counted collective indexes of organic chemical substances in this category.[34]

After chapters addressing Lavoisier's chemical nomenclature and classification, Laurent's use of geometric reasoning, and the periodic table, Dagognet turned his attention to structural organic chemistry in the final chapter of *Tableaux et langages*. Klein picks up his argument in the middle of this chapter, where he contends that "voco-structural" representation had been superseded not by written formulas, but by "the graph." Here, Dagognet presented both written chemical names and Berzelian formulas as a "stenography" that simply transcribed spoken chemical names for the purposes of memory and communication. Verbal representations, he argued, had run up against an epistemic barrier in the phenomenon of isomerism, which "called for the creation of a denser and more pictorial symbolism" and thereby "enforced the passage from the voco-structural to the perspective-pictorial," that is, to structural and stereochemical formulas.[35]

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[33] *TL*, 6–7.
[34] *TL*, 162.
[35] *TL*, 176, 179.

Klein takes issue both with the sharp distinction that Dagognet drew between verbal and visual representation, and with his unequivocal assignment of Berzelian formulas to the former category. Klein shows that the algebraic and the graphic features of these formulas were of a piece. Building on Dagognet's characterisation of structural and stereochemical formulas as semantically dense "instruments" and "tools" in *Écriture et iconographie*, Klein demonstrates that chemists of the 1820s, 1830s, and 1840s used Berzelian formulas as just such maneuverable, generative tools.[36] In this passage, she concurs with Dagognet's assessment of chemical names: they were the wrong tools for these experimental and theoretical investigations.[37]

But Dagognet did not dismiss the verbal entirely. The final chapter of *Tableaux et Langages* began by heralding systematic organic chemical nomenclature as the fulfillment of the "grand dream of Lavoisier."[38] In the passage that Klein cites, he qualified his claim that the visual had vanquished verbal representation with the prediction of "the possible revenge of an improved and streamlined 'voco-structural.'"[39] Dagognet argued that, like verbal representation before it, pictorial chemistry ran up against its own epistemic barrier in the emergence of dynamic or delocalised phenomena such as resonance. These brought about "the relative failure of the figure and the embarrassment of geometrism," resulting in a "retreat from realism" into blurring and abstraction.

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[36] Klein, *Experiments, Models, Paper Tools*, 20, 27–28.
[37] Klein, *Experiments, Models, Paper Tools*, 243–44.
[38] *TL*, 158.
[39] *TL*, 172.

Moreover, verbal representation retained another distinct advantage: names, unlike diagrams, can be alphabetised.[40] When it came to composing indexes to chemical reference works – *tables des matières*, tables of contents / tables of substances, Dagognet punned – "scientific sounds will always win out over graphical formalisms."[41] In parallel with the semiotic division between verbal and visual representations that Klein critiqued, Dagognet articulated a distinction between two sorts of paper tools: tools for investigating material substances and phenomena, and tools for documenting chemical investigations. This distinction resolves Dagognet's rather confusing oscillation throughout this chapter between praising visual and praising verbal representation. He presents them respectively as investigative and documentary paper tools, fit for different kinds of chemical practice.

Furthermore, Dagognet averred that the foundational tools of chemistry were no longer instruments of theoretical and laboratory investigation, but "the indispensable catalog, guarantor of the future."[42] Given the million and a half organic chemicals linked by diverse relationships of interest to investigators around the world, Dagognet asserted that reference works had become the foundation and condition of possibility for chemistry in general. "In our day," he wrote, "the chemist must above all constitute books of books. The universe no longer presents itself like a chart, a world map or a text: it is more comparable to an infinite library. Without a catalog, no one can find their way through it."[43] Dagognet particularly stressed that professional chemistry depended on such catalogs to avoid falling into repetition of previous work, which he characterised as a hallmark of the amateurism

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[40] *TL*, 190–94, quotations on 194.

[41] *TL*, 161.

[42] *TL*, 172.

[43] *TL*, 154–56, quotation on 155. This was likely an allusion to Jorge Luis Borges's story "The Library of Babel," published in French translation in 1952.

that chemistry had putatively left behind.[44] Indeed, he analogised the significance of information management in contemporary chemistry to its significance for business and government.[45]

Dagognet emphasised that the compilation of these indispensable books of books depended on a common vocabulary of names: systematic organic chemical nomenclature. He outlined how systematic names mapped chemical structure into prefixes, suffixes, and roots, "illuminating the depths of the substance," and, "although bound to the straight line and to duration, giving the radiant image of simultaneity, laying bare complex spatial organizations."[46] This was, Dagognet rhapsodised, the apparent realisation of "a narrow semantico-chemical parallelism, a voco-structural correspondence. For the first time, perhaps, all reality becomes speech. The entire world is word."[47] But there was a catch. Chemists had to use chemical names to communicate with each other, but the systematic names of organic compounds did not partake of the usual network of associations and experience associated with human language. As Dagognet put it:

> The neologisms lose their attachment with sensible reality, qualities, and appearances. In order to be able to go to the depths of substances, on the ocean of their relationships, it's necessary to break the moorings. The learned words, kinds of algebraic polynomials, cease to touch us. Uprooted, they address themselves only to the intelligence of structures.[48]

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[44] *TL*, 153–54, 194.

[45] *TL*, 156.

[46] *TL*, 158, 161.

[47] *TL*, 158.

[48] *TL*, 158. On the loose association between the study of mathematical structures and structuralist philosophy and social thought among Dagognet's contemporaries, see David Aubin, "The Withering Immortality of Nicolas Bourbaki: A Cultural Connector at the Confluence of Mathematics, Structuralism, and the Oulipo in France," *Science in Context* 10 (1997): 297-342.

Systematic nomenclature deputised nature itself – structural relationships among chemical substances – as guarantor of effective communication among chemists. This, Dagognet noted, was "a perilous moment for language: it blurs two antithetical goals, the social convention and the coherence of reality, the association of scientists and that of elements."[49] By making fidelity to chemical structure the necessary and sufficient criterion of a satisfactory chemical name, chemists allowed themselves to set aside concerns over consistency and legibility. In this way, individual substances acquired an "appalling plurality of names," many of which were "exact but complicated, if not unspeakable."[50] Chemists accordingly reverted to alternative names that were pronounceable and comprehensible, but did not specify the compound's structure. Here, chemical documentation had run up against its own epistemic barrier. The growth of the chemical universe ran ahead of its language, and the organic chemical analog to the periodic table surpassed the limits of human comprehension.[51]

On the other side of this rupture in chemical naming and documentation, Dagognet placed computing. "Today," he wrote, "the scientist must relinquish this insurmountable task and entrust to a computer the inventory of the vast world that he ceaselessly broadens (synthetic materials). One must pass from the old problem of order and of ordination to that of the indispensable *ordinateur* [computer]."[52] Dagognet predicted that, in the future, a computer-readable metalanguage would make sense of disparate and complex systematic names, linking them to chemical structures. With chemical names tied to such computer-

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[49] *TL*, 162.
[50] *TL*, 170.
[51] *TL*, 171.
[52] *TL*, 154.

readable representations, "the chemist will be able to 'babelize' as he pleases. A computer will register, translate, and provide information on the spot."[53] Dagognet was short on specifics about how this might work; it is hard to say whether he was yet aware of the various chemical documentation projects whose ambitions roughly aligned with his prediction.[54] Nevertheless, he suggested that computing augured a change not just in the significance of documentary paper tools but in the goals and objects of chemical practice. Chemistry, he predicted, would be "reduced partially to a third-order science of organization."[55] Its "true instrument… no longer deals with things, so to speak, but manipulates and processes knowledge or information."[56] The new chemical revolutionaries would use computers, "in a non-empirical fashion, and in a systematic and rational manner… less to search for the organization of reality than really to organize research."[57] Computer-based chemistry, Dagognet suggested, would put chemists' treasury of experimental and theoretical knowledge to work rather than seeking to augment it.

Dagognet revisited the topic of chemical representation in *Écriture et iconographie*, a semiotic tour of a wide range of topics in the history of science, art, literature, and philosophy. A core argument of the book was that the methods and achievements of science lay in the transformation of inscriptions.[58] Bruno Latour, whose career Dagognet later championed within an otherwise befuddled and hostile French academic

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[53] *TL*, 172.

[54] For a survey of such projects, see F. A. Tate, "Handling Chemical Compounds in Information Systems," *Annual Review of Information Science and Technology* 2 (1967): 285–309.

[55] *TL*, 156.

[56] *TL*, 154–55.

[57] *TL*, 195.

[58] *ÉI*, 124.

establishment, recalled that early in his training, "*Écriture et iconographie* put me on the right track: I followed it like a hunting dog, nostrils flaring."[59] Dagognet gave structural organic chemistry and its graphical representations a climactic role in his account, calling them the "Calvary of iconicity, the most formidable problem that it had to get through."[60] Focusing on the final rupture within the history that he had laid out in his previous book, Dagognet aimed to "catch in the act the slippage of a science which frees itself, which passes from the experimental to the topographic (and also the typographic), of a chemistry which turns itself into a science of writing."[61] This was a stronger claim than he had made in *Tableaux et langages* – here, Dagognet purported to describe how chemistry left experiment behind entirely to become a science focused on the creation and manipulation of graphical and textual objects.

In turning to chemistry in the book's final chapter, Dagognet drew a sharp distinction between "iconography" and "iconology." He defined iconography as methods of depiction – literally, icon-graphy, the drawing of icons. For Dagognet, iconography assumed an ontological distinction between the object of depiction and the inscription representing it, addressing the sign as a kind of thing defined by its representational function. Iconology, on the other hand, "renounced the empiricism which bathed at the same time the narrative and the engraving. It removed itself from beings, in order to grasp them better, in their constitutive architecture alone. It was no longer necessary to 'duplicate' but to replace the

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[59] Bruno Latour, "Biography of an Inquiry: On a Book about Modes of Existence," *Social Studies of Science* 43 (2013): 287–301, on 290–91. On Dagognet's support for Latour, see Hélène Mialet, "Where Would STS Be without Latour? What Would Be Missing?," *Social Studies of Science* 42 (2012): 456–61, on 457. Latour also built on Dagognet's work in his analysis of Pasteur; Bruno Latour, *The Pasteurization of France* (Cambridge, MA: Harvard University Press, 1988), 68–70.

[60] *ÉI*, 114.

[61] *ÉI*, 113.

species with their 'ideal body.'" Through a turn to iconology, Dagognet explains, some sciences "lose their experimental side and fall into that theory that is optical *stricto sensu*, that of abstract graphs…. They autonomise themselves, in order to become frankly configurational sciences, playing among the arachnoid constructions or reticulations of savants."[62] Dagognet described such objects as "abstract-concrete," on analogy with nonrepresentational art. As signifiers progressively abstract from the function of mimetic representation, they foreground their own materiality, growing concrete (and "quintessential and generative") *in themselves* as they become progressively more abstract as representations.[63] What Dagognet wanted to "catch in the act" was structural formulas becoming graphs: that is, paper tools becoming material abstractions, objects of inquiry for an autonomous chemical science.

Dagognet was not just arguing that chemistry was transforming from an experimental into a theoretical science, though he did think that this was happening too. Acknowledging this shift toward theory, he wrote: "At the limit, and more and more, the chemist will do chemistry on a blackboard and with chalk. Far from spectrometers, tubes, crystallizers, he will calculate." But Dagognet's primary interests lay elsewhere. He went on: "… in parallel, a more basic chemistry also tends to develop, which can support our conclusions: a chemistry of documents and of archives, a bookish chemistry." The proximate objects of this chemistry were neither material chemical substances nor theoretical principles, but texts. It was a "chemistry of the third degree, which makes its statements out of other statements, a sort of neo-chemistry that is textual and no longer

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[62] *ÉI*, 112–13.
[63] *ÉI*, 12.

empirical (forms) or rational (formulas)."[64] Dagognet described this as a topological (as opposed to numerical) mathematisation of chemistry: "a mathematics of graphs and matrix calculations, which allow for better understanding of the fine topology, which helps us pass from a representation that is still too realistic to one that is more abstract, that is to say more concrete."[65] It was not just that the formal expression of chemical theory was becoming topological. According to Dagognet, the objects of chemical theory were becoming topological, too.

Chemistry in the DARC

In *Écriture et iconographie*, as in *Tableaux et langages*, Dagognet tied the transformation of chemistry to the use of computers. This time, he had a particular computer program in mind: the Documentation and Automation of Research on Correlations (DARC) project of the French physical organic chemist Jacques-Émile Dubois. A brief examination of DARC will flesh out the connection between Dagognet's semiotic arguments and mid-twentieth-century chemical practice.

Dubois, a veteran of the French Resistance, an adept administrator, an enthusiastic traveler, and a polyglot, had a long and productive career in research and administration. After bolstering his hectic wartime training by means of a fellowship with Christopher Ingold in London, Dubois went on to make significant contributions in physical organic

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[64] *ÉI*, 123. Galison draws a similar connection between the fantasy of total access to information and the stability of heterogeneous scientific collectives. However, Dagognet situated his "chemistry of the third degree" apart from theory and experiment, whereas the fields of "experimenter's theory" and theorists' empirical-prediction-generating phenomenology lie between theory and experiment in Galison's account; Galison, *Image and Logic*, 42–44.

[65] *ÉI*, 130.

chemistry, especially in the fields of fast kinetics and surface chemistry.[66] He also played an active role in the French academic bureaucracy; among other positions, he directed the French national defense research agency for twelve years. But Dubois was best known for his work in "*chimie informatique*": that is, computational chemistry and chemical information.[67]

Dubois first turned to the chemistry of material abstractions to support research based on physical analytical data from UV spectroscopy. Numerous scholars have shown how the "instrumental revolution" – the widespread adoption of physical analytical instruments and methods, tailored to support rapid characterisation of chemical structures – transformed the practice of chemistry in the mid-twentieth century.[68] One of these transformations was a tendency to accord a more robust epistemic status to structural formulas, now that they could be derived through prompt instrumental methods rather than painstaking bench chemistry.[69] This was not in itself the transformation that Dagognet was trying to describe. The instrumental revolution encouraged chemists to accept structural formulas as mimetic (if schematic) representations of nano-scale chemical units in a less qualified way – to attach a physical atomism to their chemical atomism.[70] This was the opposite of the tendency away from representation and toward abstraction that

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[66] On Ingold and physical organic chemistry, see Stephen Weininger's essay in this issue.

[67] "Hommage à Jacques-Émile Dubois, un grand pionnier," *L'actualité chimique* 320–21 (2008): 7–128; Jacques-Émile Dubois, interview by Colin B. Burke, in Paris, France, on 21 January 2001 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0216) (cited hereafter as Dubois, Oral History).

[68] Peter Morris, ed., *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: Royal Society of Chemistry, 2002); Carsten Reinhardt, *Shifting and Rearranging: Physical Methods and the Transformation of Modern Chemistry* (Sagamore Beach, MA: Science History, 2006).

[69] Leo B. Slater, "Woodward, Robinson, and Strychnine: Chemical Structure and Chemists' Challenge," *Ambix* 48 (2001): 161–89.

[70] On the distinction between physical and chemical atomism, see Alan J. Rocke, *Chemical Atomism in the Nineteenth Century: From Dalton to Cannizzaro* (Columbus: Ohio State University Press, 1984).

interested Dagognet. Still, the instrumental revolution played a crucial role in enabling the emergence of chemical graphs as material abstractions: it generated large quantities of numerical data to be associated with structural formulas for chemical substances and their molecular substructures.

During the late 1950s and early 1960s, Dubois was engaged in a study of this sort, trying to work out how shifts in the UV spectra of ketones related to the intramolecular environment of the carbonyl group, the defining structural feature of ketones. This involved keeping track of hundreds of compounds with very slight structural differences, and systematically comparing the features immediately adjacent to the carbonyl group in the structural formula for each molecule. Dubois found that systematic nomenclature was not much help for this purpose. Condensed formulas (rational Berzelian formulas punctuated with parentheses to indicate branching) were more useful, but as the scale of the study grew, they too became cumbersome. Nor was Dubois satisfied with existing adaptations of chemical names and formulas designed for machine processing, such as Wiswesser Line Notation.[71]

Drawing on experience with computing gained through his role overseeing missile ranges for the French Ministry of Defense, Dubois decided to try a novel approach to representation based on the matrix mathematics of graph theory.[72] Beginning with a focal group, such as acetone in the case of the ketones that Dubois was studying, Dubois' algorithm followed the network of bonds outward, representing each non-hydrogen atom with a 1 in a matrix. Summing each column of the matrix formed a linear descriptor.

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[71] National Research Council Committee on Modern Methods of Handling Chemical Information, *Survey of Chemical Notation Systems* (Washington, DC: National Academy of Sciences, 1964).

[72] Dubois, Oral History, 13.

Additional codes linked to this descriptor accounted for heteroatoms (atoms other than carbon), bond multiplicity, and stereocenters. Dubois' representation captured the structural formula as a condensed, machine-readable *graph* – a set of atoms and a set of bonds connecting them – by abstracting from the *graphic* – the visually-suggestive structural formula.[73]

Dubois sought to establish a broader foothold for DARC as a documentary paper tool. In a retrospective interview, he recalled that he "wanted to begin in an area that had some chance of success and documentation seemed like a good place to start."[74] The advantages of DARC lay in working with large collections of structural formulas. Storing and searching for information about chemical compounds clearly required dealing with such collections, and organisations engaged in documentation possessed such collections. Dubois accordingly negotiated a joint venture with Chemical Abstracts Service to use a portion of the organisation's database of chemical structures to test and develop DARC.[75] Documentation also offered political advantages as a launching pad for the new program. Dubois told his supervisor at the defense ministry, reprising an argument that French chemists had been making for nearly a century, "France is very weak in documentation and a small country cannot be weak everywhere. We must be strong on information."[76]

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[73] Jacques-Émile Dubois, "DARC System in Chemistry," W. Todd Wipke et al., eds., *Computer Representation and Manipulation of Chemical Information* (New York: Wiley, 1974), 239–64.

[74] Dubois, Oral History, 15.

[75] J. E. Dubois, "French National Policy for Chemical Information and the DARC System as a Potential Tool of this Policy," *Journal of Chemical Documentation* 13 (1973): 8–13.

[76] Dubois, Oral History, 17. On narratives of the decline of French science, see Harry W. Paul, "The Issue of Decline in Nineteenth-Century French Science," *French Historical Studies* 7 (1972): 416–50; Robert Fox, *The Savant and the State: Science and Cultural Politics in Nineteenth-Century France* (Baltimore: Johns Hopkins University Press, 2012); and Alan J. Rocke, *Nationalizing Science: Adolphe Wurtz and the Battle for French Chemistry* (Cambridge, MA: MIT Press, 2001). On documentation and nomenclature standards as a strategy to buttress the international prestige of French chemistry, see Evan Hepler-Smith, "Nominally Rational:

At the same time, Dubois began to make use of the affordances of DARC's chemical graphs to create and study new kinds of material abstractions. He emphasised that DARC allowed for the consistent representation and study of chemical graphs that did not correspond to substances, but to substructures (sections of structural formulas) and even "hyperstructures," collections of structurally-similar compounds conceived as a single chemical entity. Dubois referred to substructures and hyperstructures as "new concepts … which meet the requirements of computer-based modern chemistry."[77] Furthermore, by enabling the chemist to select different structural subunits as the focal group around which to build the DARC graph, Dubois argued that the program answered "one of the essential needs of the chemist who must be able to perceive a structure from various angles."[78] Within DARC, the "structure" (or substructure, or hyperstructure) was the proximate object of inquiry, not the molecule. All of this reframing was to a purpose. In addition to patent searching and other documentation applications, DARC found widespread use in studies of structure-property relationships and intramolecular interactions, particularly in Europe-based work related to drug design.[79]

Dagognet saw DARC as a realisation of his speculations and predictions in *Tableaux et langages* about the direction of chemistry's development.[80] "Never has a thesis of ours received such a confirmation," he wrote, effusing that DARC "has entirely overturned modern science." Dagognet gave a detailed technical description of how DARC worked,

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Systematic Nomenclature and the Structure of Organic Chemistry, 1889-1940" (Ph.D. Diss., Princeton University, 2016), chapters 1 and 6.

[77] Dubois, "DARC System in Chemistry," 240.

[78] Ibid., 248.

[79] "Chimie informatique," in "Hommage à Jacques-Émile Dubois," 33–65.

[80] Dagognet also mentioned the parallel work of Chemical Abstracts Service, but did not discuss it in detail; *ÉI*, 125.

taking DARC's ordered graphs, its layered linear descriptors, and operations such as correlating UV spectra shifts with ketone graphs as exemplars of his argument about abstraction. The more abstract representations became, the more they became "an 'ideal body' which one can manipulate directly," and the more they supported "an informatic and automated treatment of chemical structures and their capacities."[81] DARC was less a means of grappling with individual objects than with a chemical totality; it was "able to build on populations," to realise a "general science of all representation."[82] Dagognet took Dubois's program as the realisation of the tableau – an organic chemical analog to the periodic table. This was the culmination of the history of representation that Dagognet laid out across the two books. The waxing significance of documentary paper tools within organic chemistry led to the emergence of a new, all-encompassing computer-based chemistry that took chemical graphs – material abstractions – as its proximate objects of inquiry.

Naming, algebra, and the chemical history of graph theory

In *Experiments, Models, Paper Tools*, Ursula Klein shows that structural and stereochemical formulas were not the sudden products of historical rupture that Dagognet made them out to be. Rather, these notations built upon chemists' longstanding practice of using Berzelian formulas as graphically suggestive investigative paper tools. Similarly, the material abstractions of mid-twentieth century chemistry had precedents that anticipated the transformation of chemistry that Dagognet attributed to the use of the computer. Structural formulas were already becoming material abstractions at the turn of the twentieth century, on the margins of chemistry and in allied fields. It was the shared genealogy of investigative

[81] *ÉI*, 124.
[82] *ÉI*, 128, 130.

paper tools, documentary paper tools, and mathematical graphs that made possible the emergence of programs like DARC, enabling computing to seem tailor-made for the emergence of a new, graph-based chemistry.

Chemistry's documentary paper tools and the systematic names of organic compounds were first yoked together at the 1892 Geneva Nomenclature Congress. At this four-day gathering, three dozen of Europe's leading organic chemists determined that organic compounds should have names that were fixed verbal representations of structural formulas, for use in constituting chemical indexes. Dagognet described this ideal of systematic organic chemical nomenclature as the realisation of the "grand dream of Lavoisier."[83] The designs of the convener of the Congress, the French chemist Charles Friedel, had been somewhere different. Friedel, the student and successor of Adolphe Wurtz and, like Wurtz, a staunch proponent of structure theory, advocated the use of structural formulas as investigative paper tools.[84] In his 1869 thesis, Friedel praised "the aid structural formulas offer, not only to the memory, but also to the imagination for the conduct of research" when it came to studying the constitution of substances. At the same time, he championed the "simplicity and elegance" of radical and type formulas for representing reactions in which the constitution of a core group endured unchanged. In such cases, he wrote, the use of structural formulas would be "tedious and tiresome."[85] Friedel felt similarly about chemical names. He proposed allowing chemists to select among various names expressing the structure of a given compound in different ways.

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[83] Evan Hepler-Smith, "'Just as the Structural Formula Does': Names, Diagrams, and the Structure of Organic Chemistry at the 1892 Geneva Nomenclature Congress," *Ambix* 62 (2015): 1–28.

[84] Rocke, *Nationalizing Science*.

[85] Charles Friedel, "Recherches sur les acétones et sur les aldéhydes," *Annales de la chimie et la physique* 16 (1869): 310–407, on 330.

Friedel imagined reformed chemical names, like structural formulas, serving as flexible paper tools for the purposes of laboratory investigations and pedagogy.[86]

However, other delegates – especially Adolf von Baeyer – were predominantly concerned with tailoring a system of nomenclature for the demands of one specific setting: chemical reference works. The proliferation of novel synthetic compounds, and of inconsistent ways of naming them, had made authoritative indexes such as Friedrich Beilstein's *Handbuch der organischen Chemie* increasingly vital tools of chemical research but increasingly difficult to compile and use.[87] The flexibility that made structural formulas so productive for their use as investigative paper tools was counterproductive in such settings. For constituting documentary paper tools, what was needed were fixed, stable chemical names.

Following Baeyer's recommendation, the Congress devised a collection of rules for forming a unique name for each organic compound that corresponded precisely to its structural formula. This approach to nomenclature entailed disassembling the structural formula, translating each graphical subunit into a verbal equivalent, and reassembling these prefixes, suffixes, and roots into a name, all according to well-defined rules. Listed in alphabetical order, such names classified themselves according to the structural logic by which they were formed. Dagognet referred to "algorithms, capable of recording and memorizing the invading horde" of synthetic organic chemicals as an "eventuality

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[86] On structural formulas and three-dimensional models as pedagogical tools, see Meinel, "Molecules and Croquet Balls."

[87] Michael D. Gordin, "Beilstein Unbound: The Pedagogical Unraveling of a Man and his Handbuch," in *Pedagogy and the Practice of Science: Historical and Contemporary Perspectives*, ed. David Kaiser (Cambridge: MIT Press, 2005), 11–39; Hepler-Smith, "Nominally Rational."

presupposing machine intervention."[88] However, the Geneva nomenclature, built to organise chemical information within the constraints and affordances of print, constituted just such an algorithm. It also marked a key step in the transformation of graphical instrument into chemical object. Alexander Crum Brown, one of the first chemists to use structural formulas during the 1860s, noted that names formed according to the Geneva rules "were really names of formulas rather than names of substances."[89] By this view, a gentle echo of the general wariness of "formula games" among nineteenth-century chemists, the proximate referents of Geneva names were not chemical compounds but material abstractions.

As Dagognet's analysis suggested, the application of such chemical names in reference works and elsewhere did not live up to this systematic ideal. Still, honored in the breach, the precise, rule-bound correspondence between name and structural formula was a guiding principle for the editors of Beilstein's *Handbuch*, the American Chemical Society's *Chemical Abstracts*, and other indispensable documentary paper tools of organic chemistry. These publications were staffed by a new cadre of chemists who specialised in the creation, analysis, and organisation of chemical names rather than chemical substances.[90] *Pace* Dagognet, most chemists of the 1960s did *not* spend their time assembling "books of books" with the help of computers, because specialists had already been doing so for decades before they first brought computers to bear upon this task.

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[88] *TL*, 171.

[89] Discussion of Henry E. Armstrong, "Contributions to an international system of nomenclature: The nomenclature of cycloids," *Proceedings of the Chemical Society* 8 (1892): 130–31, on 130.

[90] See, e.g., Janet D. Scott, "My Work with Chemical Abstracts," *Journal of Chemical Education* 15 (1938): 271–75.

The productivity of structural formulas as investigative paper tools drew the attention of scholars in other fields, including perhaps the most accomplished manipulators of paper tools and material abstractions during the mid-nineteenth century: Cambridge-trained mathematicians.[91] In 1857, the mathematician Arthur Cayley detailed how systematically drawn diagrams that he called "trees," made up of "knots" connected by "branches" emerging from an ultimate "root," provided a convenient accounting device for writing and checking the terms of tedious algebraic expansions.[92] A year later, in the same journal in which Cayley had described his "trees," the young Scot A. S. Couper introduced a form of chemical diagram depicting substances using atomic symbols linked by dotted lines.[93] A few years after that, Crum Brown began using structural formulas, the graphic notation of atomic symbols and bond lines that soon caught on among chemists inclined toward the emerging structure theory.[94] Crum Brown made particular use of his structural formulas as paper tools for investigating isomerism, one of the focal problems of nineteenth-century organic chemistry.[95] Coupled with rules of valence, structural formulas provided a means of enumerating assemblages of atoms in order to explain known cases of isomerism and predict new ones. For example, Kekulé backed up his hypothesis of the

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[91] Warwick, *Masters of Theory*.

[92] Arthur Cayley, "On the Theory of the Analytical Forms Called Trees," *Philosophical Magazine* 13 (1857): 172–76.

[93] Archibald S. Couper, "On a New Chemical Theory," *Philosophical Magazine* 16 (1858): 104–16.

[94] Rocke, *Image and Reality*, 118–60.

[95] A. Crum Brown, "On the Theory of Isomeric Compounds," *Transactions of The Royal Society of Edinburgh* 23 (1864): 707–19.

hexagonal structure of benzene by counting the number of distinct isomers of various substitution products that his structure implied should exist.[96]

In the mid-1870s, Cayley applied his algebraic paper tool to this chemical problem. By examining the properties of his diagrams, given restrictions corresponding to the valence rules, he developed algebraic functions for predicting the number of organic compounds of various sorts. The number of distinct trees of *n* knots (in Cayley's terms) in which each knot connected to at most four others corresponded to the number of unique saturated hydrocarbon isomers with *n* carbon atoms.[97] The number of unique knots within such a tree corresponded to the number of distinct isomers of a substitution product of the hydrocarbon, such as alcohols.

During the 1880s and 1890s, several chemists eagerly took to Cayley's graphical tools for enumeration, experimenting with their use on various isomer-counting problems.[98] However, the investigative paper tool was only as useful as the problems that it could address were interesting. After the turn of the century, structure theory *per se* was no longer a topic of active debate. Isomer-counting remained an important technique for interpreting experimental data in determining the structures of specific compounds, but chemists could typically sketch each such isomer by hand rather than resorting to calculation. It became less and less obvious what general principles isomer-counting might prove; the results of chemical combinatorics lost touch with the practical capacities and

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[96] August Kekulé, "Note sur quelques produits de substitution de la benzine," *Bulletin de la classe des sciences, Académie Royale de Belgique* 19 (1865): 554.

[97] Arthur Cayley, "On the Mathematical Theory of Isomers," *Philosophical Magazine* 47 (1874): 444–47; Arthur Cayley, "On the Analytical Forms Called Trees, with Applications to the Theory of Chemical Combinations," *Report of the British Association for the Advancement of Science* 45 (1875): 257–305.

[98] Henry R. Henze and Charles M. Blair, "The Number of Isomeric Hydrocarbons of the Methane Series," *Journal of the American Chemical Society* 53 (1931): 3077–85, on 3077–79.

concerns of chemists. "For example," admitted one mathematician reflecting on a 1932 paper, "no chemist *really* needs to know that the number of alkanes having 60 carbon atoms is 22,158,734,535,770,411,074,184."[99] The same year, a member of the editorial board of the *Journal of the American Chemical Society* critiqued a series of isomer-counting papers, writing "I have always considered Cayley's paper as of only interest as a curiosity only [*sic*] and of no practical of theoretical value in Chemistry…. It is something like counting the number of leaves on a tree. Unless it is connected with some important idea, the work appears to me quite useless."[100] To mathematicians more interested in applied counting than in its theoretical stakes in another domain, the isomer problem remained interesting. Indeed, a large proportion of the 1930s research behind the Hungarian mathematician George Pólya's enumeration theorem – a generalised approach to counting – addressed concrete problems of counting chemical isomers.[101] The theorem is widely regarded as one of the more significant achievements of twentieth-century mathematics and became a foundation for applications of combinatorics in computer science, but it was of little interest to contemporaneous chemists.[102] When chemists took interest in isomer combinatorics once more, a method stood ready at hand.[103]

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[99] Ronald C. Read, "The Legacy of Pólya's Paper," in George Pólya, *Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds* (New York: Springer, 1987 [1937]), 96–135, on 124. Italics in original.

[100] Noyes to Lamb, 14 Sept 1932, William A. Noyes Papers, 15/5/21, University of Illinois Archives, Urbana, IL, Box 11, Folder General Correspondence, 1932.

[101] Pólya, *Combinatorial Enumeration*; George Pólya, "Tabelle der Isomerenzahlen für die einfacheren Derivate einiger cyclischen Stammkörper," *Helvetica Chimica Acta* 19 (1936): 22–24; Frank Harary et al., "Pólya's Contributions to Chemical Enumeration," in Alexandru T. Balaban, ed., *Chemical Applications of Graph Theory* (New York: Academic Press, 1976), 11–24.

[102] Read, "The Legacy of Pólya's Paper."

[103] For example, Robert K. Lindsay et al., *Applications of Artificial Intelligence for Organic Chemistry: The DENDRAL Project* (New York: McGraw-Hill, 1980).

Cayley's friend and collaborator James Joseph Sylvester perceived a deeper connection between organic chemistry and mathematics. At first, he, too, framed his engagement with these intersections between disciplines as mathematical contributions to chemistry. In 1869, he suggested that, by classifying algebraic forms, he might also be "solving a problem of the Chemistry of the Future," Brodie's calculus of chemical operations.[104] After chemists lost interest in Brodie's theory, and through discussions and correspondence with Crum Brown, Sylvester decided that the link between chemistry and mathematics lay instead in structural formulas.[105] Sylvester cited structural organic chemistry as one of the signal applications for his principle of colligation – a mode of mathematical theorising about domains whose subject matter could be expressed as units connected by discrete links, such as the atoms and bonds of structural formulas. Even when its objects were depicted geometrically, Sylvester explained that such a theory was "not spatial but logical … in one word of *connection* in the abstract." In language similar to and perhaps inspired by that of structural chemists distinguishing their chemical atomism from physical atomism, Sylvester wrote that his mathematical theory of chemistry operated on structural formulas but took "no account of magnitude or position; geometrical lines are used, but have no more real bearing on the matter than those employed in genealogical tables have in explaining the laws of procreation." He argued that his account lent clarity and rigor to structure theory and "an *a priori* ground for the formula of the saturated

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[104] James Joseph Sylvester, "Outline Trace of the Theory of Reducible Cyclodes [1869]," in *The Collected Mathematical Papers of James Joseph Sylvester*, vol. 2 (Cambridge: Cambridge University Press, 1908), 663–88, on 680.

[105] James Joseph Sylvester, "On an Application of the New Atomic Theory to the Graphical Representation of the Invariants and Covariants of Binary Quantics," *American Journal of Mathematics* 1 (1878): 64–104, on 89–90.

hydro-carbons C_nH_{2n+2}."[106] If chemists' conceptions of valence and structure continued to be borne out in experimental investigations, Sylvester predicted, his theory would "introduce a firm basis of predictive science into chemistry."[107]

Soon thereafter, Sylvester decided that he had gotten it backwards: the real potential in the connections between mathematics and structural organic chemistry was not in the mathematisation of chemistry but in the application of chemistry to mathematics. As organic chemists developed the concept of valence and determined structural formulas for myriad compounds, Sylvester contended in 1878, they had unknowingly been amassing "an untold treasure of hoarded algebraical wealth."[108] Sylvester detailed how structural formulas, which Sylvester now referred to as "chemical graphs" or "chemicographs," could be applied to the representation of abstract algebraic objects called invariants.[109] As he extended the analogy and generalised these chemical graphs – "mere translations into geometrical forms of trains of priorities and sequences having their proper habitat in the sphere of order" – he began referring to them simply as "graphs."[110] Sylvester's "chemistrization of algebra" (as historian Karen Parshall has described it) had little immediate impact on either chemistry or algebra.[111] However, mathematicians took a keen

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[106] James Joseph Sylvester, "On Recent Discoveries in Mechanical Conservation of Motion [1874]," in *Collected Mathematical Papers*, vol. 3, 7–25, on 23–24.

[107] James Joseph Sylvester, "On the Plagiograph *aliter* the Skew Pantigraph [1875]," in *Collected Mathematical Papers*, vol. 3, 26–34, on 28.

[108] Sylvester, "Application of the New Atomic Theory," 87.

[109] Sylvester, "Chemistry and Algebra," *Nature* 17 (1878): 284; Sylvester, "Application of the New Atomic Theory."

[110] Sylvester, "Application of the New Atomic Theory," 79

[111] Karen Hunger Parshall, "Chemistry Through Invariant Theory? James Joseph Sylvester's Mathematization of the Atomic Theory," in *Experiencing Nature: Proceedings of a Conference in Honor of Allen G. Debus*, ed. Allen G. Debus, Paul Harold Theerman, and Karen Hunger Parshall (Boston: Kluwer, 1997), 81–111.

interest in Sylvester's graphs – fashioned out of chemists' paper tools – as objects of mathematical investigation in their own right.[112]

Sylvester's graphs were not just tools for the practice of theory but entities about which one could have a theory. In *Theory of Finite and Infinite Graphs*, regarded as the founding text of the field of graph theory, the mathematician Dénes Kőnig cited Sylvester as the originator of these mathematical objects.[113] Graph theory became the foundation for the design and analysis of algorithms, data structures, and other major topics in the applied mathematics of computing (not to mention electrical engineering, social network analysis, and myriad other fields). Meanwhile, in the decade following World War II, large chemical firms and publishers of chemical reference literature began developing machine-based methods and machine-readable versions of systematic nomenclature to support the compilation and organisation of more and more information about more and more chemical substances. The independent fields of mathematical graph theory and chemical documentation, each rooted in late nineteenth-century studies of structural formulas, converged in the work of Dubois and like-minded scientists and engineers in the 1950s and 1960s.[114] As Alexandru Balaban, one of the principal exponents of the recombination of chemistry and graph theory, put it, "Having chemistry as one of the breeding grounds, graph theory is well adapted for solving chemical problems… [that is,] for an 'inverse osmosis,' namely for chemistry to profit from the progress of graph theory."[115] The material

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[112] Norman Biggs, E. Keith Lloyd, and Robin J. Wilson, *Graph Theory 1736-1936* (Oxford: Clarendon Press, 1976), 67.

[113] Dénes Kőnig, *Theory of Finite and Infinite Graphs*, trans. Richard McCoart (Boston: Birkhäuser, 1990 [1936]).

[114] Willett, "Chemoinformatics: A History."

[115] Balaban, *Chemical Applications of Graph Theory*, vii.

abstractions that computers were built to manipulate had been modeled from the start on chemists' structural formulas. The "Copernican revolution" (as Dagognet had put it) embodied in DARC and systems like it was not just a rupture in the history of chemistry, but also a return to this shared origin.

Conclusion: Scriptural chemistry

Needless to say, chemistry never became a third-order science of organisation, occupied with documents, graphs, and writing rather than materials, experiments, and visual representations. Computers have become tools for extending experimentation, in the form of simulations, and for providing ever more spatially and visually suggestive renderings of chemical substances.[116] The capacity for the material world to defy exact prediction, to demand experimental engagement, and to resist easy manipulation remains a defining feature of the chemical sciences.[117] As Ursula Klein and Bernadette Bensaude-Vincent have pointed out, by taking representation as the essence of chemistry, Dagognet was unable to account for the material practices that underwrite the industrial and productive aspects of chemistry. The waxing interest in just those features of chemistry that Dagognet neglected, coupled with Dagognet's essayistic style and meager engagement with other scholarship, contributed to the relative lack of attention by historians and philosophers to his studies of chemistry.[118]

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[116] Thus the chemist Pierre Laszlo describes the computer as affording chemists a "return to naive realism"; Laszlo, *Parole des choses*, 76–78. See Pio Garcia, "Computer Simulations and Experiments: In Vivo–in Vitro Conditions in Biochemistry," *Foundations of Chemistry* 17 (2015): 49–65; Joachim Schummer, "Gestalt Switch in Molecular Image Perception: The Aesthetic Origin of Molecular Nanotechnology in Supramolecular Chemistry," *Foundations of Chemistry* 8 (2006): 53–72.

[117] Bensaude-Vincent and Simon, *Chemistry: The Impure Science*.

[118] Klein, *Experiments, Models, Paper Tools,* 232; Bensaude-Vincent, "Dagognet et la chimie."

But *part* of chemistry did transform in the manner that Dagognet described. It may be most productive to take his work as a philosophical history of "scriptural chemistry."[119] Scriptural chemistry comprises the aspects of chemistry that involved writing, reading, organising, and manipulating representations of chemical structure. It runs from the "formula games," nomenclature rules, and chemical reference works of the late nineteenth century to the computer-based structure-activity correlations and bibliographic databases of the mid-twentieth century and beyond. If the study of "objects of chemical inquiry" requires historians and philosophers "to shift back and forth in their studies between chemists' representation and material referents," as Klein and Carsten Reinhardt have described, the study of scriptural chemistry shows that representations sometimes *are* the material referents of chemists' inquiries.[120] It encompasses the fields of chemical documentation and cheminformatics. It has its own modes of practice that, though not quite theory and not quite experiment, are nevertheless socially sanctioned as chemistry, and that, as Dagognet pointed out, are crucial supports for more readily recognised forms of experimental and theoretical practice.[121] At the turn of the twentieth century, one could hardly be an organic chemist without using Beilstein's *Handbuch*; a present-day organic chemist could hardly avoid engaging at least indirectly with the Chemical Abstracts Service Registry.[122] Such studies of chemistry's documentary paper tools and material abstractions would enrich the history of modern chemistry and could create an opportunity for

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[119] *ÉI*, 130.

[120] Klein and Reinhardt, *Objects of Chemical Inquiry*, vii–viii.

[121] In this sense, scriptural chemistry was "marginal and necessary," as Galison writes of the technique of Monte Carlo simulation in particle physics; Galison, *Image and Logic*, 689–780 (quotation on 732.)

[122] Gordin, "Beilstein Unbound"; Roger J. Schenck and Kevin R. Zapiecki, "Back to the Future: CAS and the Shape of Chemical Information to Come," in *The Future of the History of Chemical Information*, ed. Leah Rae McEwen and Robert E. Buntrock (New York: Oxford University Press, 2014), 149–58.

interchange with emerging scholarship on the relationship between reading, writing, and experiment in early modern alchemy.[123] They would also add a crucial missing thread to emerging scholarship on "science in the archives" and on the historical genealogy of data science and its computer-based tools and techniques.[124]

Four insights drawn from Dagognet's work are particularly productive places to start. The first is that chemical documentation is a field of chemical practice worthy of historians' attention as such. In print and on machines, chemical reference works have been indispensable documentary paper tools, and they have histories, objects, and methods of their own. The second is Dagognet's concept of the abstract-concrete: the materiality of chemical formulas and notation (on a page, a screen, or a disk) tends to be more apparent when these inscriptions represent their chemical referents in a more abstract manner. The topographic and typographic are closely connected. The third, which Dagognet does not mention but which the second half of this essay suggests, is that the investigative paper tools of chemists were made into material abstractions in their application for purposes other than inquiries into chemical phenomena. Mathematicians and editors, not experimental or theoretical organic chemists, made structural formulas into chemical graphs. Finally, the chemistry of material abstractions reveals a previously unexplored dimension of methodological pluralism in the history of chemistry. Chemists investigating individual substances used formulas as investigative paper tools. Scientists who wished to learn something about large collections of chemical substances – hundreds of very slightly different ketones, in Dubois' case, or all of the isomers composed of a certain set of atoms,

[123] For example, Jennifer M. Rampling, "Transmuting Sericon: Alchemy as 'Practical Exegesis' in Early Modern England," *Osiris* 29 (2014): 19–34.

[124] Daston, *Science in the Archives*; Aronova, von Oertzen, and Sepkoski, "Data Histories."

for Cayley and Pólya – stepped away from chemical substances and theories and turned their attention to material abstractions. Interpreted in this sense, Dagognet's tableau – "the totality of substances, along with the properties of each of them and the multiplicity of relationships that ties it to the others" – is not a Borgesian fantasy of an infinite library or a life-sized map of the chemical world. Rather, it is a different way of knowing chemicals, at the scale of many chemical substances rather than one. In each of these senses, for a significant minority of chemists since the late nineteenth century, it has been "enough, somehow, to write, to write better, in order to know."[125]

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[125] *ÉI*, 130