

Molecular Bureaucracy: Toxicological Information and Environmental Protection

Evan Hepler-Smith

Email: heplers@bc.edu

Abstract: Legal and political claims about environmental chemicals typically address such substances on a molecule-by-molecule basis. This essay argues that this approach is not determined solely by the nature of chemicals. Rather, it is the product of legal structures, administrative procedures, regulatory lists, information systems, and nomenclature conventions, which I collectively term “molecular bureaucracy.” This essay traces the development of molecular bureaucracy, a global framework of environmental governance grounded in American regulatory infrastructure, and its political and environmental consequences. It does so by following the history of PFASs, synthetic chemicals in widespread use since the 1950s whose toxicity has become a prominent subject of research and public concern since the late 1990s. Molecular bureaucracy originated in a classification system based on molecular identity developed to make chemical information accessible to the late-nineteenth century synthetic chemicals industry. It came to structure environmental law and politics through, first, the efforts of 1960s US policymakers to render toxic hazards subject to government control through computer-based information coordination, and second, a vision of chemical holism within the nascent US EPA and the Toxic Substances Control Act, which sought to accommodate the global environment to rational administration by aggregating diverse toxic hazards and reframing them as abstract chemical substances. The history of molecular bureaucracy offers valuable insights for present-day efforts to ground toxic substances scholarship and politics in alternative conceptions of environmental chemicals.

The limitations of regulations to control toxic environmental chemicals have turned out to be as persistent as these long-lived pollutants themselves. Numerous factors have constrained what can be known and what can be done about toxic chemicals within the regulatory regimes of the mid-twentieth through early twenty-first centuries: protection of corporate confidentiality, the calculus of risks and benefits, regulatory capture, political culture, ongoing histories of colonization and discrimination, out-and-out deception, the circulation of toxic substances across political boundaries, and the challenges posed by long-term, low-dose, and/or intergenerational toxicity, among others. Material-, place-, and

body-based histories show how environmental toxicants have defied the assumptions of regulatory models. Historians and social scientists have also documented how members of contaminated communities and scientist-advocates have pressed alternative claims about which chemicals are toxic, what makes a chemical safe, and who should be held responsible for chemical safety and toxicity.¹

This essay poses a complementary question that cuts across such histories of chemical toxicity: what kinds of things count as chemicals? On the one hand, chemicals are material substances situated in networks of biogeochemical, economic, and political relations. By this view, a chemical “is defined by its metamorphoses, that is, by its past and its future,” as the pioneering organic chemist Charles Gerhardt wrote in 1850.² On the other hand, in the context of legal, regulatory, and political claims about environmental toxicity, chemicals are abstract molecules: networks of atoms and bonds, always and everywhere the same, defined independently of their origins, effects, and fate. Molecular identity is usually taken as either a precise representation of nature—what chemicals

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Notes

¹ For overviews of this extensive scholarship, see Max Liboiron, Manuel Tironi, and Nerea Calvillo, eds., “Special Issue: Toxic Politics,” *Social Studies of Science* 48 (2018): 331–445; Liza Gross and Linda S. Birnbaum, eds., “Challenges in Environmental Health: Closing the Gap between Evidence and Regulations” *PLOS Biology* 15 (2017), <https://collections.plos.org/challenges-in-environmental-health>; Nicholas Shapiro and Eben Kirksey, eds., “Chemo-Ethnography,” *Cultural Anthropology* 32 (2017): 481–513; Jody A. Roberts and Nancy Langston, eds., “Toxic Bodies/Toxic Environments: An Interdisciplinary Forum,” *Environmental History* 13 (2008): 629–703; Gregg Mitman, Michelle Murphy, and Christopher C. Sellers, eds., “Landscapes of Exposure: Knowledge and Illness in Modern Environments,” *Osiris* 19 (2004).

² Quoted in John Hedley Brooke, “Laurent, Gerhardt, and the Philosophy of Chemistry,” *Historical Studies in the Physical Sciences* 6 (1975): 405–29, on 424.

really are—or as an artifact of the reductive lens of chemistry. Neither is quite correct. Though grounded in properties of matter and generalizations of chemists, molecular identity was purpose-built for *bureaucratic* purposes.

Since the 1960s, pathways for addressing the hazards of environmental chemicals have run through molecular bureaucracy: the global complex of legal structures, administrative procedures, regulatory lists, information systems, and nomenclature conventions that render toxic environments tractable to regulatory politics on a molecule-by-molecule basis. Within molecular bureaucracy, molecular identity is the defining feature of chemical substances; chemical substances are the agents of environmental toxicity; and environmental toxicity is to be controlled through coordinated information systems. Molecular bureaucracy takes environmental concerns tied to phenomena spanning scales from the local and sensible (noxious smells; mysterious illnesses) to the global and statistical (worldwide hotspots of persistent pollutants) and channels them into universalizing claims about abstract, homogeneous molecules. Despite this disconnection—or, rather, because of it—molecular bureaucracy is a bulwark of environmental chemicals regulation. Molecular bureaucracy contributes to what STS scholar Michelle Murphy terms “regimes of perceptibility” and “domains of imperceptibility”; it enables regulators, scientists, and industry and environmental advocates to cut through the complexity of environmental toxicity to mobilize evidence associated with molecules—and to efface evidence of other kinds.³ It supports well-

³ Michelle Murphy, *Sick Building Syndrome and the Problem of Uncertainty: Environmental Politics, Technoscience, and Women Workers* (Durham: Duke University Press, 2006), 9–10. On this point, see also Sara Shostak, *Exposed Science: Genes, the Environment, and the Politics of Population Health* (Berkeley: University of California Press, 2013).

intentioned but stigmatizing “damage-centered” research that reduces people and lands to chemical-by-chemical summations of harmful exposures.⁴ It engenders a persistent pattern of “chemical whack-a-mole,” in which chemicals of concern are replaced by substitutes that turn out to be no less hazardous.⁵ Abstractions matter.⁶ Molecular bureaucracy has material consequences.

Consider the per- and polyfluoroalkyl substances (PFASs), chemicals used in Teflon manufacturing, waterproof and stainproof fabrics, food packaging, and firefighting foams. Since the late 1990s, community activism, citizen science, and litigation has brought considerable scientific and public attention to one such substance, perfluorooctanoic acid (PFOA). Manufacturers long suspected PFOA might be environmentally persistent and toxic, based on internal studies; however, limited disclosure requirements and strong corporate confidentiality protections in the US Toxic Substances Control Act (TSCA) enabled them to conceal these concerns. Journalists and social scientists aptly take PFOA toxicity as a case of regulatory weakness, corporate misconduct, and grassroots knowledge.⁷ But this is not the end of the story. PFOA is the kind of object—a chemical substance of “a particular molecular identity”—that laws like TSCA address. In contrast, considered in terms of molecular identity, the PFASs comprise thousands of such chemicals—including chemicals introduced as substitutes for PFOA. The “intractable, potentially never-ending chemicals management issue” posed by the PFASs is a product of

⁴ Eve Tuck, “Suspending Damage: A Letter to Communities,” *Harvard Educational Review* 79 (2009): 409–28.

⁵ Ken Geiser, *Chemicals without Harm: Policies for a Sustainable World* (Cambridge, MA: MIT Press, 2015).

⁶ William Cronon, *Nature’s Metropolis: Chicago and the Great West* (New York: Norton, 1991), 268.

⁷ Lauren Richter, Alissa Cordner, and Phil Brown, “Non-Stick Science: Sixty Years of Research and (in)Action on Fluorinated Compounds,” *Social Studies of Science* 48 (2018): 691–714.

their persistence within molecular bureaucracy as well as within bodies and environments.⁸

Drawing on historical and ethnographic studies of ontology and of information infrastructures, this essay complements historical scholarship on environmental toxicity focused on materials, places, and bodies. Contextual studies of ontology attend to how, even within a putatively universal domain like that of chemical substances, multiple different kinds of entities have constituted suitable subjects for scientific, legal, political, and cultural claims in different places, times, and communities of practice.⁹ Scholars of information infrastructure show how ways of dividing up the world are articulated within information technologies and bureaucracies. The entrenchment of categories obscures their contingency; “ontology, whatever else it is, is usually just forgotten infrastructure.”¹⁰ For example, nutrients (as the constituents of food) and pathogens (as the agents of agricultural blight) emerged alongside institutionalized regulatory and technoscientific interventions.¹¹ In STS terminology, such ontologies and bureaucracies are co-produced. Nutrients and pathogens exist apart from classification practices, but they nonetheless limn and are limned by bureaucracy.¹²

⁸ Zhanyun Wang et al., “A Never-Ending Story of Per- and Polyfluoroalkyl Substances (PFASs)?,” *Environmental Science & Technology* 51 (2017): 2508–18, on 2511.

⁹ Ian Hacking, *Historical Ontology* (Cambridge, MA: Harvard University Press, 2002); Annemarie Mol, *The Body Multiple: Ontology in Medical Practice* (Durham: Duke University Press, 2002).

¹⁰ Geoffrey C. Bowker and Susan Leigh Star, *Sorting Things Out: Classification and Its Consequences* (Cambridge, MA: MIT Press, 1999); quotation in John Durham Peters, *The Marvelous Clouds: Toward a Philosophy of Elemental Media* (Chicago: University of Chicago Press, 2015), 38.

¹¹ Xaq Frohlich, “The Informational Turn in Food Politics: The US FDA’s Nutrition Label as Information Infrastructure,” *Social Studies of Science* 47 (2017): 145–71; Julie Guthman, *Wilted: Verticillium Dahliae in the Making and Unmaking of California’s Strawberry Industry* (forthcoming).

¹² Sheila Jasanoff, *States of Knowledge: The Co-Production of Science and Social Order* (New York: Routledge, 2004), 2.

Following this insight into the molecular world draws attention to the historicity of chemical interactions and identity. The historical agency of chemical substances lies not only in nanoscale chains of causation, but in the systems through which people interpreted and propagated these effects.¹³ If the politics of environmental chemicals is a game of chess, and chemicals are the pieces, environmental laws the rules, and methods of toxicology and advocacy the strategies, then molecular bureaucracy is the game board. The pieces exist apart from the board, but the board structures how players make sense of the pieces.

This essay follows the historical emergence of molecular bureaucracy from its origins in the research and development activities of the late-nineteenth century German synthetic chemicals industry, through efforts to render toxic hazards subject to government control in the 1960s US, to its present-day political and environmental consequences. Thematically, I address three trends that came together—and into conflict—within molecular bureaucracy: first, molecular identity as an approach to managing information about chemicals; second, government information coordination initiatives that addressed toxic hazards via computer-based information systems; and third, a substance-by-substance chemical holism envisioned as a means of accommodating the global environment to rational administration. Outside of molecular bureaucracy and obscured by it, chemicals continued to exist otherwise. Recent scholarship addresses chemicals as residues of the past in the environmental present, vectors of power and responsibility, and constituents of physical, social, and political “metabolic flows,” echoing the chemist

¹³ Pace the “neo-materialist” emphasis on the historical agency of chemicals as “things-in-and-of themselves” described in Timothy J. LeCain, *The Matter of History: How Things Create the Past* (New York: Cambridge University Press, 2017), 16.

Gerhardt's conviction that a chemical is defined by its past and future.¹⁴ The conclusion suggests how the history of molecular bureaucracy might inform efforts to ground the history and politics of toxicity in such alternative understandings of environmental chemicals.

Constructing Molecular Identity

The catalogs, lists, and databases that provide access to information about the properties of chemicals nearly always organize this information on a substance-by-substance basis. These substances—the thousands or millions of entries enumerating the objects that any given chemical fact may be a fact about—are typically defined in terms of molecular identity: a specific set of atoms linked by a specific network of bonds. There are exceptions, as we will see. But by default, information about chemicals comes attached to the molecular identities expressed in names like “perfluorooctanoic acid.”

These catalogs, lists, and databases are not just archives of scientific knowledge. Like laboratories and the field, these archives are sites where data is gathered for further analysis, for administering laws, and for justifying political claims. The way an information resource itemizes the basic units of a scientific domain shapes what can be done with the data it contains; recognizing this, their creators tended to design them with specific purposes in mind. Re-used for other purposes or in other domains, they carry with them the capacities for which they were originally designed.¹⁵ This is a well-documented feature

¹⁴ Soraya Boudia et al., “Residues: Rethinking Chemical Environments,” *Engaging Science, Technology, and Society* 4 (2018): 165–78; Michelle Murphy, “Alterlife and Decolonial Chemical Relations,” *Cultural Anthropology* 32 (2017): 494–503; David Biggs, “Following Dioxin’s Drift: Agent Orange Stories and the Challenge of Metabolic History,” *International Review of Environmental History* 4 (2018): 7–31.

¹⁵ Lorraine Daston, *Science in the Archives* (Chicago: University of Chicago Press, 2017).

of environmental sciences such as paleontology, climatology, and biological systematics.¹⁶ It is true of chemistry as well. The authoritative reference works of the chemical sciences were created at the turn of the twentieth century to support the growth of the synthetic chemicals industry by promoting the development of new chemical products. Taken up as tools for other purposes, including documenting and controlling the toxicity of chemical products, they carried with them the propensity to enable the proliferation of new chemical substances and new uses of known ones. As the historian Hannah Landecker observes, twentieth-century chemical technologies ushered society into “a strange time of controlling prior modes of control.”¹⁷ The enumeration of chemicals according to molecular identity is part of the reason why.

When it was first introduced in the late nineteenth century, this fixed conception of the individuality of chemical substances went against the grain. Then, as now, chemistry was characterized by its multiplicity.¹⁸ Chemists treated diagrams and mental images of molecules not as depictions of nano-scale reality, but as “paper tools” and imaginative resources.¹⁹ The value of molecular thinking lay in its capacity to organize empirical

¹⁶ 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; Paul N. Edwards, *A Vast Machine: Computer Models, Climate Data, and the Politics of Global Warming* (Cambridge, MA: MIT Press, 2010); Staffan Müller-Wille and Isabelle Charmantier, “Lists as Research Technologies,” *Isis* 103 (2012): 743–52.

¹⁷ Hannah Landecker, “Antibiotic Resistance and the Biology of History,” *Body & Society* 22 (2016): 19–52, on 44. See also Hannah Landecker, “Postindustrial Metabolism: Fat Knowledge,” *Public Culture* 25 (2013): 495–522, tracing the manufacturing-oriented genealogy of information-oriented biochemical studies of metabolism, a history analogous and perhaps connected to the industrial genesis of chemical information systems.

¹⁸ Bernadette Bensaude-Vincent, “Chemists without Borders,” *Isis* 109 (2018): 597–607.

¹⁹ Ursula Klein, *Experiments, Models, Paper Tools: Cultures of Organic Chemistry in the Nineteenth Century* (Stanford: Stanford University Press, 2003); Alan J. Rocke, *Image and Reality: Kekulé, Kopp, and the Scientific Imagination* (Chicago: University of Chicago Press, 2010).

relationships while bridging different research programs, theories of matter, and scales of chemical identity. Yet when a group of distinguished chemists gathered in Geneva in 1892 to devise international standards for naming chemicals, they came up with an algorithmic method for transforming abstract patterns of atomic interconnections into fixed, structure-based systematic chemical names. From the start, commentators pointed out that this idea of molecular identity was impoverished at best, often frankly misleading, and lacked the flexibility that was so useful in teaching, developing theories, and conducting experiments. That was the point. Systematic names and the conception of molecular identity they embodied were not designed for teaching, theory, or experimentation, but to put lists of tens of thousands of chemical substances into a chemically meaningful alphabetical order, making it possible to compile and search long lists of chemicals efficiently and reliably.

For the emerging synthetic chemicals industry, this was a decisive advantage. Coal tar, a waste product of municipal gas production, had become a proven source of lucrative new synthetic dyes; dye-manufacturing byproducts were themselves beginning to yield synthetic pharmaceutical fortunes. A chemical naming system grounded in molecular identity enabled editors to distill the mass of journal articles and patents addressing synthetic chemicals into compound-by-compound entries in meticulously ordered reference works. Paid for largely by industry support, these publications became crucial tools for industrial research, enabling researchers to search for promising chemicals in the library as well as the laboratory. As of the mid-twentieth century, the world's foremost such tool was the American Chemical Society publication *Chemical Abstracts*, which put the

entirety of chemical science and industry, including toxicology, pharmacology, and industrial hygiene, into molecule-by-molecule order.²⁰

The PFASs typified the kinds of chemicals whose development *Chemical Abstracts* chronicled and supported. During World War II, the Manhattan Project enlisted academic and industrial chemists to develop fluorine-containing synthetic chemicals for use in nuclear weapons production. When this research was declassified after the war's end, the chemical firms 3M and DuPont quickly filed patents on these fluorochemicals, whose "almost unbelievable" properties—strong acidity, stability, oil-, water-, and grease-resistance—promised to yield valuable consumer products and industrial processes.²¹ As with many chemical patents, they did not claim an individual molecular identity, but general structural features associated with useful properties: "fluorocarbon acids and derivatives," in the case of the 3M patent that encompassed PFOA. In the index of *Chemical Abstracts*, this broadly-defined chemical entity was split into systematic names expressing individual molecular identities, scattered across multiple index volumes in accordance with alphabetical order.²² Neither the lumping of the patent claim nor the splitting of the index entries was an intrinsically more accurate way to define the identity of chemical substances. Rather, each textual instrument defined chemical identity based on different aspects of the material properties of chemicals to serve different bureaucratic purposes.

²⁰ 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.

²¹ Albert R. Diesslin and Edward A. Kauck, "Fluorocarbon Acids and Derivatives," United States Patent US2567011, issued 4 September 1951 (quotation at 8:51). On the history of PFASs and other fluorochemicals, see Rebecca Altman, "Time Bombing the Future," forthcoming in *Aeon*; Richter, Cordner, and Brown, "Non-Stick Science."

²² *Chemical Abstracts*, index to vol. 41-50 (1947-1956), subject index (1960).

As global chemistry and chemical industries grew, so did the chemical literature and the challenge of keeping reference works up to date. The bottleneck in producing chemical indexes was translating chemical names into diagrams and back, verifying that, for example, *perfluorooctanoic acid*, *perfluorocaprylic acid*, *F-octanoic acid*, and the eye-glazing, wrist-numbing *2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid* all referred to the molecular identity of PFOA.²³ Mechanical methods of information management offered alternatives to molecular identity. Several inventors devised punched-card and computer-based schemes that identified chemicals according to selected structural features and that could flexibly lump or split the identities of chemicals like the fluorocarbon acids in the 3M patent.²⁴

However, the value of *Chemical Abstracts* was tied to molecular identity, via decades' worth of back issues and indexes (dozens of volumes, tens of thousands of pages) already ordered in this manner. In the late 1950s, the directors of this publication hatched a plan to address its mounting production costs, consolidate its dominant position, and provide profitable new services via an electronic database: the Chemical Abstracts Service (CAS) Registry. Borrowing a technique developed at DuPont, the CAS Registry expressed molecular identity in the form of computer-readable tables of atoms and bonds. Each of these entries was assigned a short code called a Registry Number (figure 1). Registry Numbers said nothing about chemical structure; they merely identified a Registry entry.

²³ The nomenclature of PFASs continued to cause confusion through the 2010s. See discussion of naming conventions in Interstate Technology Regulatory Council, "PFAS Fact Sheets," <https://pfas-1.itrcweb.org/fact-sheets/>, accessed 6 December 2018.

²⁴ Evan Hepler-Smith, "Paper Chemistry: François Dagognet and the Chemical Graph" *Ambix* 65 (2018): 76–98.

Plenty of index entries addressed substances of interest to *Chemical Abstracts* readers whose molecular identity was indeterminate or beside the point (from “asbestos” to “Zwieback”). Unlike systematic names, these common terms did not slow down the index-making process appreciably; editors could handle such entries manually. They were left off the computer-based Registry.²⁵

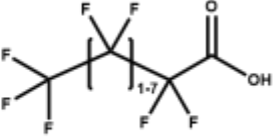
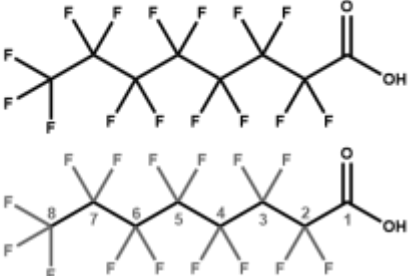
Structural formulas	<p style="text-align: center;">PFASs</p>  <p style="text-align: center;">$F_{2n+1}C_n$</p>	<p style="text-align: center;">PFOA</p> 
Names/descriptions	<p style="text-align: center;">fluorocarbon acids</p> <p>“fully fluorinated saturated non-cyclic monocarboxylic acids which have from four to ten carbon atoms in the molecule and are represented by the formula $C_nF_{2n+1}COOH$”</p>	<p style="text-align: center;">perfluorocaprylic acid C8</p>
Systematic names	<p>n/a (considered as one chemical); many (considered as many molecules)</p>	<p style="text-align: center;">perfluorooctanoic acid F-octanoic acid 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid</p>
CAS Registry Number	<p>n/a (considered as one chemical); many (considered as many molecules)</p>	<p style="text-align: center;">335-67-1</p>

Figure 1. Left: structural formulas (diagrams), name, and description of the substances claimed in a PFAS patent granted to 3M in 1951, treated as a single product encompassing a range of molecular identities. Right: PFOA, a molecular identity encompassed by that patent, with systematic names and Registry Number. Each systematic name expressed a specific molecular identity, but systematic names allowed for synonyms, whereas CAS Registry Numbers were unique. Credit: Author.

²⁵ Evelyn Constance Powell, “A History of Chemical Abstracts Service, 1907-1998,” *Science & Technology Libraries* 18, no. 4 (2000): 93-110.

The simplicity of Registry Numbers was the key to their enormous importance. They enabled verification of molecular identity without interpreting cumbersome systematic names, and they established the CAS computer system as the authoritative clearinghouse for addressing molecular identity in this way. The CAS Registry would thus make chemical information more broadly accessible (especially to non-chemists). It would also entrench molecular identity as the framework for information about the myriad, ubiquitous chemical products of industrial modernity—including information about their toxicity.

Coordinating toxicological information

“If we are going to live so intimately with these chemicals,” wrote Rachel Carson in *Silent Spring*, “eating and drinking them, taking them into the very marrow of our bones—we had better know something about their nature and their power.”²⁶ For US federal policymakers during the early 1960s, emerging evidence of the long-term, low-dose hazards of pesticides, fallout, cigarettes, and drugs made existing practices of labeling “adulterants” and setting threshold values for acute exposure seem grossly insufficient.²⁷ In principle, the US government knew plenty about the toxicity of drugs, pesticides, and other chemicals. Government-sponsored research had cultivated toxicity as a useful property for protecting human health against microbes, for waging war, and for controlling weeds and

²⁶ Rachel Carson, *Silent Spring* (Boston: Houghton Mifflin, 2002 [1962]), 17.

²⁷ On pesticides and fallout: Soraya Boudia, “From Threshold to Risk: Exposure to Low Doses of Radiation and Its Effects on Toxicants Regulation,” in *Toxicants, Health and Regulation since 1945*, ed. Soraya Boudia and Nathalie Jas (London: Pickering & Chatto, 2013), 71–87. On drugs: Daniel P. Carpenter, *Reputation and Power: Organizational Image and Pharmaceutical Regulation at the FDA* (Princeton: Princeton University Press, 2010), 228–297. On cigarettes: Allan M. Brandt, *The Cigarette Century: The Rise, Fall, and Deadly Persistence of the Product That Defined America* (New York: Basic Books, 2007), 211–40. On workplace exposures vis-à-vis environmental health: Christopher C. Sellers, *Hazards of the Job: From Industrial Disease to Environmental Health Science* (Chapel Hill: University of North Carolina Press, 1997).

pests.²⁸ Emerging toxic harms—in many cases caused by the same chemicals—still came as a surprise. Policymakers concluded that effective governance of these hazardous industrial technologies would require coordinated information technologies.

The framing of the challenge of toxic substances in terms of information coordination followed a broad pattern in the US (and around the world) during the 1950s and 1960s, in which policymakers sought to apply information technology to the challenges of public administration.²⁹ As the historians Jennifer Light and Jacob Hamblin have pointed out, federal lawmakers and administrators tended to apply the terms in which they grappled with the military and geopolitical crises of the early Cold War to the social and environmental crises of the period.³⁰ Prominent among these was a “closed-world discourse” in which pervasive, world-spanning hazards could be managed through massive, integrated, computer-based information systems.³¹ The historian Xaq Frohlich has shown that this trend extended to food and nutrition. Regulations requiring “imitation” labels on packaged foods whose ingredients deviated from traditional norms gave way to mandatory quantification and labeling of nutrition information. This “informational turn” brought together the authority of science, the right to know, the protection of health, and the food industry’s desire to eliminate the consumer-detering “imitation” label. In turn,

²⁸ Edmund Russell, *War and Nature: Fighting Humans and Insects with Chemicals from World War I to Silent Spring* (New York: Cambridge University Press, 2001).

²⁹ Ronald R. Kline, “Cybernetics, Management Science, and Technology Policy: The Emergence of ‘Information Technology’ as a Keyword, 1948-1985,” *Technology and Culture* 47 (2006): 513–35.

³⁰ Jennifer S. Light, *From Warfare to Welfare: Defense Intellectuals and Urban Problems in Cold War America* (Baltimore: Johns Hopkins University Press, 2003); Jacob Darwin Hamblin, *Arming Mother Nature: The Birth of Catastrophic Environmentalism* (New York: Oxford University Press, 2013).

³¹ Paul N. Edwards, *The Closed World: Computers and the Politics of Discourse in Cold War America* (Cambridge, MA: MIT Press, 1996), 7, 10.

neoliberal trends in food beginning in the 1990s were grounded in nutrition labeling and the information infrastructure that supported it.³² The same is true of the turn toward a politics of environmental toxicity based on right-to-know laws, publicly accessible electronic databases, and market-based regulatory mechanisms that aim to empower individuals rather than constrain businesses—what anthropologist Kim Fortun terms the “informating of environmentalism.”³³ Administratively and technologically, both the politics of individual choice and that of collective action for environmental justice rest on systems built to support government control.

During the early 1960s, plans to address toxic hazards through information coordination sprouted up throughout the US federal government. In the Senate, Hubert Humphrey’s Subcommittee on Reorganization and International Organizations seized upon the thalidomide affair and *Silent Spring* to launch inquiries into interagency management of information regarding the toxicity of drugs, pesticides, and other chemical products. The President’s Science Advisory Committee launched its own investigation, as did the National Bureau of Standards and the National Research Council. All concluded that the key to effective management of the toxic byproducts of modern civilization lay in an “automated Federal network of information,” linking data gathered by government agencies and published in scientific literature into a “much more coordinated and more complete computer-based file.” Such a network was to support chemical regulation, the public’s right

³² Frohlich, “The Informational Turn in Food Politics.”

³³ Kim Fortun, “From Bhopal to the Informating of Environmentalism: Risk Communication in Historical Perspective,” *Osiris* 19 (2004): 283–96.

to know about toxic hazards, researchers' and responders' access to hazard information, and the anticipation of hazards through computer modeling.³⁴

The "most crucial element" of this system, the studies emphasized, was that it connect disparate information on a chemical-by-chemical basis.³⁵ Since each agency's portion of the "total body of chemical and biological information" might be relevant for the others, "a comprehensive network can service effectively workers in all fields which deal with the biological consequences of any environmental component."³⁶ The President's Science Advisory Committee encapsulated this collection of data in the term "toxicological information," defined as "information descriptive of the effects of chemicals on living organisms or their component subsystems."³⁷ This defined the content of toxicological information in capacious, flexible terms ("effects," "organisms," "subsystems"), but the subject of toxicological information was invariably an individual chemical. The pressing question became how these chemical-by-chemical links could be forged.

This question was also of considerable interest to CAS directors, who were beginning to look to federal patronage as a source of funds for building their Registry. To their consternation, some lawmakers proposed a centralized, government-based system,

³⁴ Quotations from "Interagency Drug Coordination," report of Subcommittee on Reorganization and International Organizations, Senate Committee on Government Operations (Washington: USGPO, May 5, 1966), 5; "Handling of Toxicological Information," report of the President's Science Advisory Committee (originally published in 1966), in *Symposium on the Handling of Toxicological Information*, ed. George J. Cosmides (Springfield, VA: NTIS, 1978), 201–223, on 212. See also National Research Council, *Survey of Chemical Notation Systems* (Washington: National Academies, 1964); Ethel C. Marden, *A Survey of Computer Programs for Chemical Information Searching*, National Bureau of Standards Technical Note 85 (Washington: Department of Commerce, 1961).

³⁵ "Interagency drug coordination," 6.

³⁶ *Ibid.*, 100–101, quoting a Public Health Service report to the subcommittee.

³⁷ "Handling of Toxicological Information," 204.

possibly managed by the Army. However, grant-makers at the National Science Foundation preferred to rely on the existing bibliographic enterprises of non-governmental scientific organizations like the American Chemical Society.³⁸ The National Research Council committee, of which the CAS research director was an influential member, determined that the core of the national chemical information network should be computer-based representations of molecular identity tied to a system of registry numbers—the specifications of the CAS Registry. Committee members recognized that this approach would cause difficulties for dealing with chemical substances like asbestos, materials of toxic concern that could not be represented in terms of molecular identity. Nevertheless, noting that most users of chemical information already depended on CAS, the committee determined that the CAS Registry should play this key role in the federal network. In this way, the system that CAS developed for computer-based chemical bibliography became the least-common-denominator framework for organizing the US government's toxicological data.³⁹

Based on these recommendations, CAS secured several million dollars in grants and contracts to develop the Registry system. Over the following decade, CAS Registry Numbers became the keystone of an information infrastructure spanning the US government and stretching around the world. CAS contributed to programs at the National Library of Medicine (NLM), the FDA, the National Institute for Occupational Safety and Health, the

³⁸ Dale B. Baker, 9 June 1997 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0160), 21–24, 55, 72–73.

³⁹ *Conference on Mechanical Processing of Chemical Information, March 5-8, 1964* (Washington: National Academies, 1964); Paul D. Olejar, "Coping with the Data Flood: The Federal Role in Chemical Registry," *Chemical Heritage* 12 (1995): 7–8.

National Cancer Institute, and the Atomic Energy Commission, among other agencies. The American Chemical Society-based CAS also exported the Registry system, bringing Registry Numbers to toxicological information initiatives of governmental, nongovernmental, and intergovernmental organizations around the world.⁴⁰ By the mid-1970s, a computing expert at the National Institutes of Health remarked, this “emerging pattern of international cooperation seems to have ensured the fact that all molecular structure files will be linked to the CAS Registry Number in the future.” Scientists should accordingly “think of data as being linked to the body of chemical information” by the Registry Number, a “universal identifier.”⁴¹

Though Registry Numbers interconnected these lists via molecular identity, their contents remained chemical products: drugs, or food additives, or pesticides, or some other class of substances that raised toxicological concerns according to its context of use. Drug toxicity had to account for the method of administration and the effects of (putatively) inactive ingredients. Pesticide registrations addressed formulations, mixtures of chemical compounds within dispersal media such as fuel oil. Just as molecular identity brought together literature references from different fields of chemistry in *Chemical Abstracts*, it linked bodies of data about disparate products held by different agencies as a networked information system. Information coordination meant that data about toxicity could travel. When this data traveled into a domain of administration that aimed to address the *total*

⁴⁰ Cosmides, *Symposium on the Handling of Toxicological Information*.

⁴¹ Richard J. Feldmann, “The Design of Computing Systems for Molecular Modeling,” *Annual Review of Biophysics and Bioengineering* 5 (1976): 477–510.

environment, the meaning of toxicological information—and the molecular identities that held it together—changed.

Chemical Holism at the EPA

Like chemistry, the environment is (among other things) a bureaucratic domain. Fields such as ecosystems science, genetic toxicology, and environmental risk assessment came into being alongside envirotechnical disasters, tools, and politics, most often involving nuclear or chemical technologies.⁴² New laws and agencies aiming to govern the environment as a whole drew on emerging fields of environmental science and supported their development as an epistemic foundation for effective administration. This holistic administrative rationality was among the primary bases for the establishment of the US Environmental Protection Agency (EPA) and the Toxic Substances Control Act (TSCA). The EPA and TSCA were to eliminate gaps and redundancies that arose from separate laws and agencies addressing toxic pollutants in the air, waterways, landfills, or workplaces. They would do so by reconceiving environmental contamination in terms of chemicals, rather than releases, emitters, or sites. Reorganizing monitoring, research, and regulation around individual chemicals, wherever they might be, was to provide a foundation for holistic knowledge and control of the global environment. This chemical holism provided a mechanism (though not always an effective one) for addressing substances that previously

⁴² Scott Frickel, *Chemical Consequences: Environmental Mutagens, Scientist Activism, and the Rise of Genetic Toxicology* (New Brunswick, NJ: Rutgers University Press, 2004); Laura J. Martin, "Proving Grounds: Ecological Fieldwork in the Pacific and the Materialization of Ecosystems," *Environmental History* 23 (2018): 567–592; Soraya Boudia, "Managing Scientific and Political Uncertainty: Environmental Risk Assessment in a Historical Perspective," in Soraya Boudia and Nathalie Jas, eds., *Powerless Science?: Science and Politics in a Toxic World*, (New York: Berghahn Books, 2014), 95–112; Sara B. Pritchard, "An Envirotechnical Disaster: Nature, Technology, and Politics at Fukushima," *Environmental History* 17 (2012): 219–43.

slipped through the cracks of environmental toxicology and regulation, including PFOA. Yet efforts to capture global wholes in comprehensive lists tend to fall into a kind of “reductive holism,” as the historian Joanna Radin has described.⁴³ Chemical holism had its own set of cracks.

The government agencies that enforced media-based pollution control laws were included in the federal network of toxicological information. Here, in addition to linking databases of chemical products, the abstract molecules represented by CAS Registry numbers became objects of scientific inquiry in themselves. Extending methods of industrial hygiene beyond the factory, toxicologists were beginning to work with the concept of “body burden,” the overall accumulation of a chemical within a human or other organism. Ecologists were tracing global flows of chemicals as emissions from different sources merged, diverged, and traveled across media. Both relied on the work of enterprising instrument manufacturers, who created tools for rapid characterization of chemical samples in terms of molecular identity; these instruments further encouraged chemists to represent their objects of inquiry in this way.⁴⁴ In 1967, a Johnson administration task force argued that only through “research... specifically aimed at a given chemical compound to determine toxicity” could the public come to grips with environmental health hazards. The task force accordingly recommended systematic

⁴³ Joanna Radin, *Life on Ice: A History of New Uses for Cold Blood* (Chicago: University of Chicago Press, 2017), 9, 182.

⁴⁴ Peter Morris, ed., *From Classical to Modern Chemistry: The Instrumental Revolution* (Cambridge: Royal Society of Chemistry, 2002); Angela N. H. Creager, “Human Bodies as Chemical Sensors: A History of Biomonitoring for Environmental Health and Regulation,” *Studies in History and Philosophy of Science Part A* (2018); Angela N. H. Creager, *Life Atomic: A History of Radioisotopes in Science and Medicine* (Chicago: University of Chicago Press, 2013).

investigation of “the toxicity of all chemical compounds which may come into contact with individuals, either directly or through environmental links.”⁴⁵

At the same time, administrative liaisons and efficiency-minded observers were beginning to see the separate agencies responsible for air pollution, water pollution, solid waste, pesticides, radioactive materials, and occupational toxins as a patchwork ridden with “imbalance, overlap, and neglect.”⁴⁶ The Ash Council, a Nixon administration committee on government reorganization, seized on the pollution control bureaucracy as “Federally-sponsored irrationality”—a ripe target for its program of administrative reform (especially for a White House keen to bolster its bona fides on the popular issue of environmental protection). The group proposed bringing together these diverse programs within a single administrative unit, the Environmental Protection Agency, with subunits responsible for monitoring, research, standard-setting, enforcement, and assistance across all media. Such an organization, a product of the systems thinking that shaped both ecology and management during the postwar decades, was intended to enable administrators to “come to grips with the environment as an entity.”⁴⁷

The keystone of this holistic approach to environmental protection was the chemical substance. “What is needed,” wrote a key staff member, based on his experience overseeing the budget for environmental programs under the previous administration, “is a

⁴⁵ Task Force on Environmental Health, *A Strategy for a Livable Environment: A Report to the Secretary of Health, Education, and Welfare* (Washington: USGPO, 1967), 20.

⁴⁶ *Environmental Quality: The First Annual Report of the Council on Environmental Quality* (Washington: USGPO, 1970), 24.

⁴⁷ Marc Karnis Landy, Marc J. Roberts, and Stephen R. Thomas, *The Environmental Protection Agency: Asking the Wrong Questions* (New York: Oxford University Press, 1990), 22–45. Quotation in President’s Advisory Council on Executive Organization, Memorandum for the President on Federal Organization for Environmental Protection, April 29, 1970, <https://archive.epa.gov/epa/aboutepa/ash-council-memo.html>, accessed on 6 July 2018.

Federal agency with responsibility for determining the health effects of all such substances, setting standards for human exposure to them, registering and approving new chemicals, and monitoring the course of such substances in the environment, thus tracing the sources of human exposure.”⁴⁸ The EPA was to consider “‘total body burden’—that is, how much of a given substance an individual is exposed to whether it comes from air, water, or land.”⁴⁹ This approach leveraged principles from ecology and toxicology (which, historian Linda Nash argues, “reproduce[d] the world in the image of the early twentieth-century factory”) for administrative purposes: “Standard-setting, monitoring, and control can often be done more efficiently and rationally if attention is focused on the particular substance.”⁵⁰ In principle, data about particular substances could then be recombined to assess the real-world conditions of exposure to many different chemicals at once, via the toxicological principles of synergism, potentiation, and antagonism. By *dis*-embedding pollution from place, chemical holism was to provide a basis for rational environmental bureaucracy.

However, existing pollution control programs had administrators, budgets, relationships with interest groups, and congressional patrons. Bowing to expedience, the Nixon administration transferred these programs intact into the EPA.⁵¹ The vision of administrative rationality grounded in chemical holism was carried forward within the EPA’s research division, whose staff of chemists and information technologists built a series of agency-wide information systems organized and interconnected by CAS Registry

⁴⁸ J. Clarence Davies, *The Politics of Pollution* (New York: Pegasus, 1970), 199.

⁴⁹ *Environmental Quality*, 25-26.

⁵⁰ Linda Nash, “Purity and Danger: Historical Reflections on the Regulation of Environmental Pollutants,” *Environmental History* 13 (2008): 651–58, on 656; Council on Environmental Quality, *Toxic Substances* (Washington: USGPO, 1971), 22.

⁵¹ Landy, Roberts, and Thomas, *The Environmental Protection Agency*, 30-37.

Numbers.⁵² For the fledgling agency pummeled from all sides by litigation, these information systems cast environmental encounters in terms of discrete chemicals tractable to legally defensible decisions.⁵³ For example, the EPA settled a National Resources Defense Council lawsuit over enforcement of the Clean Water Act by specifying molecular identities for 129 “priority pollutants” to be earmarked for scrutiny.⁵⁴ Chemical holism was a philosophy for administrative reform; information coordination was a political path of least resistance. Together, they transformed molecular identity from an interface interconnecting different sources of chemical information into an ontology defining what counted as a chemical.

The Toxic Substances Control Act embodied this philosophy. Drafted alongside initial plans for the EPA, the act was to provide legislative grounding for the Agency’s chemical holism. A report explaining the rationale for the initial 1971 bill noted that chemicals of concern such as mercury, cadmium, and polychlorinated biphenyls (PCBs) had been released into the environment through diverse pathways. “No agency has considered itself completely responsible for all such substances in all media”; thus diffuse warning signs were ignored and lessons of toxic crises went unlearned.⁵⁵ Amid the divergent

⁵² Stephen R. Heller, “The History of the NIST/EPA/NIH Mass Spectral Database,” *Today’s Chemist at Work* 8 (1999): 45–46, 49–50.

⁵³ William D. Ruckelshaus, “Stopping the Pendulum,” *Environmental Toxicology and Chemistry* 15 (1996): 229–32.

⁵⁴ Claudia Copeland, “Toxic Pollutants and the Clean Water Act: Current Issues,” Congressional Research Service Report 93-849 ENR (1993).

⁵⁵ Council on Environmental Quality, *Toxic Substances*, v, 11–14, 21 (quotation on v); J. Clarence Davies, 30 October 2009 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0640), (cited hereafter as “Davies oral history”) 5–13. On mercury and PCBs, respectively, see Brett L. Walker, *Toxic Archipelago: A History of Industrial Disease in Japan* (Seattle: University of Washington Press, 2010), 137–175; Ellen Griffith Spears, *Baptized in PCBs: Race, Pollution, and Justice in an All-American Town* (Chapel Hill: University of North Carolina Press, 2014).

perspectives of administrators, environmentalists, and industry lobbyists, one provision of the proposed law attracted general enthusiasm: a section calling for the creation of a standard classification and information system for all chemical compounds. An EPA staffer called this an “essential device” for the implementation of the bill. A Sierra Club representative thought it was the best part of the bill, affirming that “legislation which aims to control hazardous and toxic substances should include all chemical substances and should work toward developing a standard classification system of chemical compounds.” The Manufacturing Chemists’ Association also approved of this information-based plan — provided trade groups were consulted in its development of.⁵⁶ This information system—the Chemical Substances Inventory, a list of all chemical substances in commercial use in the United States—was the centerpiece of EPA toxic substances policy under TSCA, which became law in 1976. By this time, negotiations with the Commerce Department and Congress had diluted the other powers TSCA conferred upon the agency. The final law provided neither resources to conduct toxicity testing, power to require manufacturers to test their own products, nor leeway to make rules without substantial evidence of toxicity and exposure. What it did mandate was creation of the Inventory. By cataloguing “existing chemicals,” the Inventory channeled agency attention toward “new chemicals”; under TSCA, this was the “foundation upon which all toxic substances control will be based.”⁵⁷ As an EPA staff member involved in rolling out the law pithily put it, “Inventory gets you [the

⁵⁶ *The Toxic Substances Control Act of 1971 and Amendment: Hearings* (Washington: USGPO, 1972), 27, 90, 114–115, 294.

⁵⁷ Davies oral history, 9–14; Frederick H. Siff, “Inventory Information in the Chemical Abstract Service,” in *2nd Annual ADP Conference* (Washington: EPA, 1977), H-11–13, on H-11.

list]. Separates old from new. No new PCBs, boom.”⁵⁸ As for chemicals already in use, the Inventory’s chemical holism was to ensure that apparently unrelated concerns about the same existing chemicals would add up. As Paul Edwards has written about global climate models, the TSCA Chemical Substances Inventory was to enclose “the real green world... within the closed world.”⁵⁹

This did not always make for an easy fit. For one thing, the act permitted manufacturers to claim the molecular structure of a substance as a trade secret, preventing the EPA from disclosing its molecular identity in the publicly accessible Inventory. For another, as commenters on the bill’s initial draft pointed out, defining chemical substances in terms of molecular identity excluded some substances of grave concern, such as asbestos.⁶⁰ The final act accordingly addressed not only “substance[s] of a particular molecular identity,” but also “any combination of such substances occurring in whole or in part as a result of a chemical reaction or occurring in nature.”⁶¹ Once the initial Inventory was complete, this latter group, chemicals of unknown or variable composition, complex reaction products, and biological materials—“UVCBs,” in agency jargon—amounted to nearly 10,000 chemicals, about a sixth of the entire list.

The chemical holism of TSCA thus legally obliged the EPA to keep track of chemical substances that could not adequately be represented in terms of molecular identity. The CAS Registry, grounded in tables of atoms and bonds representing molecular identity,

⁵⁸ James V. Aidala, 20 May 2010, (Philadelphia: Chemical Heritage Foundation, Oral History Transcript), 28.

⁵⁹ Edwards, *The Closed World*, 350. See also Edwards, *A Vast Machine*.

⁶⁰ *The Toxic Substances Control Act of 1971*, 130, 224.

⁶¹ *Legislative History of the Toxic Substances Control Act* (Washington: USGPO, 1976), 4. This definition excluded deliberate mixtures of chemicals, for which each constituent was treated as a separate chemical substance.

offered no way of doing so. But by 1977, CAS Registry Numbers were thoroughly integrated into information systems at EPA and many other government agencies, and relationships between CAS staff and federal bureaucrats ran equally deep. EPA staff engaged CAS to adapt the Registry system to fit the needs of the Inventory. Sacrificing consistency to expedience, CAS assigned Registry Numbers to these UVCBs, adding an asterisk flagging these numbers as exceptions to the molecular order of the Registry.⁶²

From the 1970s through the 2010s, chemical regulatory regimes around the world expanded, contracted, transformed, diverged, and interlinked, at scales from the local to the global, through processes of institutional change co-constituted with major political, scientific, and environmental developments. Diverse organizations added to an ever-growing thicket of molecule-by-molecule lists and registers, nearly all of which relied on Registry Numbers as a taken-for-granted standard for defining what counted as chemicals and sharing toxicological information. The precaution-based approach of the EU's 2007 REACH regulations is grounded in molecule-by-molecule dossiers of toxicological data.⁶³ The Lautenberg Chemical Safety Improvement Act, a 2016 US law that revised TSCA, kept the law's chemical-by-chemical orientation in place.

Molecular identity, designed as a bibliographic tool, was made the basis for the CAS Registry, and then for the coordination of toxicological information, and then for chemical holism at the EPA and beyond. At each step, administrators and policymakers recognized the shortcomings of molecular identity but bowed to the bureaucratic convenience of

⁶² J. P. Moosemiller, A. W. Ryan, and R. E. Stobaugh, "The Chemical Abstracts Service Chemical Registry System. VIII. Manual Registration," *Journal of Chemical Information and Computer Sciences* 20 (1980): 83–88.

⁶³ Henri Boullier, "Autoriser pour interdire: La fabrique des savoirs sur les molécules et leurs risques dans le règlement européen REACH" (Ph.D. dissertation, Université Paris-Est, 2016).

Registry Numbers. The information infrastructure tying toxicological information to molecular identity and Registry Numbers became steadily broader and more deeply entrenched. This is not to say that building such systems was easy. The EPA official who oversaw the implementation of TSCA remarked, “the choice of using the Chemical Abstract Services [CAS] means of identification [...] led to all kinds of technical issues and nomenclature issues that took huge amounts of time and resources.... It just has nothing to do with protecting health and safety.”⁶⁴ Information systems had opportunity costs. They absorbed attention and resources that might have gone toward the other epistemic and political challenges posed by TSCA and similar laws. As it was, protecting health and safety in fact had everything to do with time- and resource-intensive nomenclature issues. This is molecular bureaucracy.

Material Consequences

The perfluorocarbon acids and related compounds—PFASs—exemplify the sorts of chemicals that the EPA and TSCA were supposed to bring under control. They were synthetic, numerous, anonymous, and subject to many different uses, releases, and human exposures. By the time that TSCA was passed, PFAS chemicals had realized their miraculous promise as constituents of consumer products and industrial processes. PFASs were used in fast-food containers, microwave popcorn bags, Gore-Tex water-resistant clothing, Scotchgard fabric protector, stain-resistant carpets, firefighting foams, electronics manufacture, film processing, and most especially in the production of Teflon and other

⁶⁴ Steven D. Jellinek, (Philadelphia: Chemical Heritage Foundation, Oral History Interview #0653 (2010), 7. (First ellipsis in transcript, second ellipsis added.)

fluorine-containing polymers.⁶⁵ Beginning in 1951, DuPont used a fluorocarbon surfactant, purchased from 3M, to produce Teflon at its Washington Works factory along the Ohio River near Parkersburg, West Virginia. Between the 1960s and the 1980s, DuPont and 3M toxicologists found evidence linking exposure to the substance with cancer, liver disease, and birth defects in lab animals; it appeared in the blood of factory workers and in local water supplies. A 1981 survey showed that two of seven children born to Washington Works employees exposed during pregnancy suffered birth defects. DuPont established exposure limits for employees, reassigned women workers to minimize exposure, and purchased land for off-site disposal of Teflon-production waste. At the urging of company lawyers, DuPont researchers explored possible substitutes, but decided not to pursue their development.⁶⁶

Meanwhile, PFOA—the molecular identity represented by the Registry Number 335-67-1—entered the regulatory sphere as an existing chemical, as did dozens of other PFAS chemicals included in the TSCA Chemical Substances Inventory. In principle, this made these PFASs accessible to regulatory scrutiny; in practice, it provided a bulwark against regulators’ attention. Between processing a constant stream of new chemical applications and gathering evidence on high-profile chemicals of concern such as asbestos and formaldehyde, EPA staff had little time to go searching for toxic needles in the haystack of existing chemicals. When it came to new chemicals, the EPA was able to draw on molecular bureaucracy to make data breed data. When new chemical applications arrived

⁶⁵ “Occurrence and Use of Highly Fluorinated Substances and Alternatives,” KEMI (Swedish Chemicals Agency) Report 7/15 (2015).

⁶⁶ Callie Lyons, *Stain-Resistant, Nonstick, Waterproof, and Lethal: The Hidden Dangers of C8* (Westport, CT: Praeger, 2007); Richter, Cordner, and Brown, “Non-Stick Science.”

absent toxicity information, EPA staff scoured information systems organized according to molecular identity and knit together by Registry Numbers, identified existing compounds with similar molecular structures, and gathered data relevant to their toxicity, persistence, and bioaccumulation. This method, termed structure-activity relationship modeling, yielded rough and ready estimates of potential hazards, which the agency used to justify permitting the new chemical to come to market or requiring further testing.⁶⁷ However, litigation-wary regulators did not apply this approximate method to the higher threshold of evidence regarding existing chemicals.⁶⁸ And while TSCA required that manufacturers report new evidence that an existing chemical posed an unreasonable risk to health or the environment, the law did not specify what evidence was reportable or how to ensure it was reported. DuPont kept its PFAS findings to itself.

These hazards came to light via sick livestock, dead wildlife, a creek full of chemical froth, an irate farmer, a determined lawyer, and persistent journalists, activists, and community members.⁶⁹ As concerns mounted about the Teflon-making chemical variously known as APFO, PFOA, Fluorad FC-143, C8, and ammonium perfluorooctanoate, molecular bureaucracy cut through the terminological confusion, focusing attention on the molecular identity of PFOA. Molecular bureaucracy also enabled these toxicological concerns to propagate across other products associated with PFOA, such as additives for stainproofing carpets. Between 2002 and 2018, PFOA was the subject of more than 4,000 peer-reviewed

⁶⁷ Charles M. Auer, J. Vincent Nabholz, and Karl P. Baetcke, "Mode of Action and the Assessment of Chemical Hazards in the Presence of Limited Data: Use of Structure-Activity Relationships (SAR) under TSCA, Section 5," *Environmental Health Perspectives* 87 (1990): 183–97.

⁶⁸ Charles M. Auer, 23 April 2010, (Philadelphia: Chemical Heritage Foundation, Oral History Transcript), 6–12.

⁶⁹ Lyons, *Stain-Resistant, Nonstick, Waterproof*; Richter, Cordner, and Brown, "Non-Stick Science."

research articles, most addressing its toxicology, all indexed by CAS and tied together via the registry number 335-67-1. Instruments and databases designed to detect signatures of molecular identity located PFOA in environments and organisms around the world.⁷⁰

Paired with revelations of the firms' long-undisclosed concerns, this evidence added up to a multi-million dollar fine for DuPont and tort settlements of just under a billion dollars each for DuPont and 3M, with further cases pending.⁷¹ The EPA negotiated a voluntary plan for chemical firms to phase out PFOA by 2015. The United Nations Persistent Organic Pollutants Review Committee has recommended a global ban on the production and use of PFOA under the Stockholm Convention.⁷² A lot can happen when so much attention is focused on one molecule.

Yet focus may entail myopia. As Michelle Murphy and the historian Gregg Mitman have pointed out, against the white noise of low-level exposure to diverse molecules, insistence on associating toxicity with molecular identity has produced uncertainty about chemical causation and rendered social and political causes of chronic disease imperceptible.⁷³ This, too, was in part a consequence of molecular bureaucracy, in which new evidence about toxicity could only be incorporated into the "body of chemical and biological information" (a telling metaphor) if it came attached to a molecule. And while the

⁷⁰ Wang et al., "A Never-Ending Story," 2510.

⁷¹ Marc Reisch, "DuPont, Chemours Settle PFOA Suits," *Chemical & Engineering News* 95, no. 8 (February 20, 2017): 5; Marc S. Reisch, "3M to Pay \$850 Million to Settle Fluorosurfactants Lawsuit" 96, no. 9 (February 26, 2018): 12.

⁷² "Two more toxic chemicals recommended to be eliminated as UN scientific committee paves way for ban on widely-used PFOA," Stockholm Convention on Persistent Organic Pollutants, press release of 21 Sept 2018, <http://www.brsmeas.org/?tabid=7685>, accessed 25 Oct 2018.

⁷³ Gregg Mitman, *Breathing Space: How Allergies Shape Our Lives and Landscapes* (New Haven: Yale University Press, 2007); Murphy, *Sick Building Syndrome*.

ability to search and group molecules by structural similarity offered a crucial (if legally dubious) resource for broadening the purchase of such evidence, accommodations for trade secrets and UVCBs compromised this capacity. Consider Surflon S-111, a fluorosurfactant used to manufacture the polymer PVDF, a chemical cousin of Teflon. Surflon S-111 comprised multiple molecular identities; it was registered on the TSCA Inventory as “carboxylic acids, C7-13, perfluoro, ammonium salts” (Registry Number 72968-38-8*).⁷⁴ Its name clearly announces that it is a PFAS chemical, but as a UVCB chemical without a well-defined molecular structure, it was an isolated individual within the databases of molecular bureaucracy—even though it literally encompassed PFOA (figure 2).

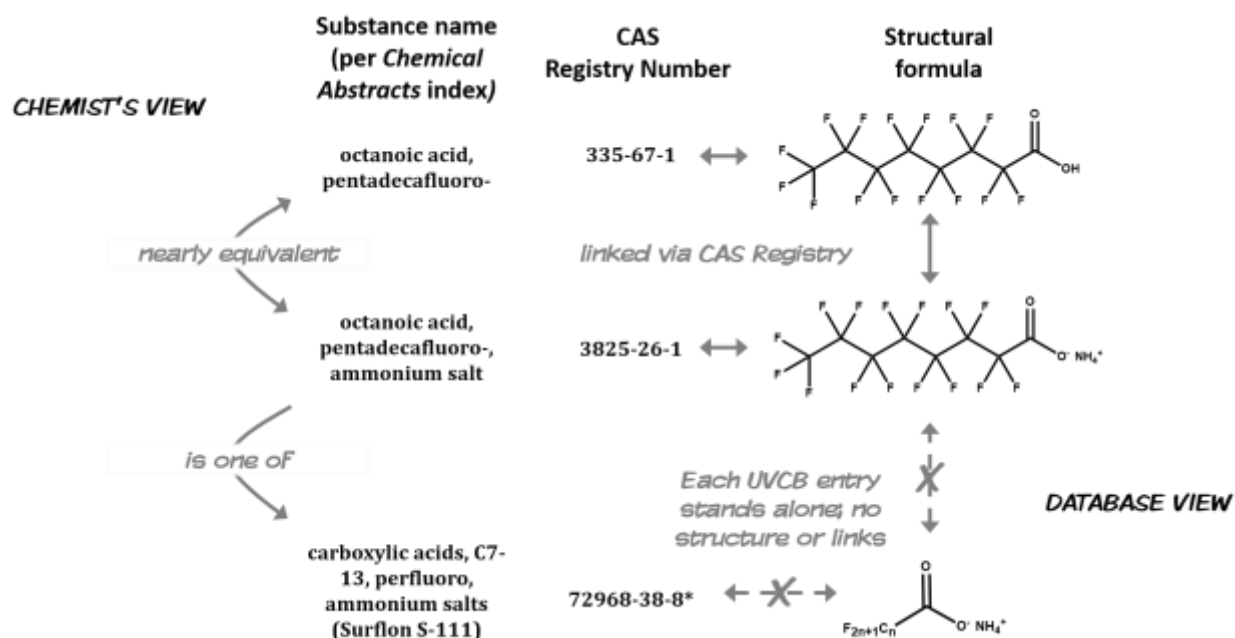


Figure 2. A chemist’s understanding of three entries for PFAS chemical substances on the TSCA Chemical Substance Inventory, vis-à-vis their handling within

⁷⁴ *Toxic Substances Control Act Chemical Substance Inventory: Cumulative Supplement* (Washington: EPA, 1980), 172. “C7-13” represented the number of carbon atoms that might be contained in molecules making up the substance.

databases linked to the CAS Registry. The Registry Numbers for the two compounds at top are linked to computer-based representations of their molecular identities, which capture their close structural relationship. The UVCB chemical at bottom is on the TSCA Inventory but cannot be situated in structural relation to the others, since its Registry Number is not linked to a specific molecular identity. Credit: Author.

Environmental toxicologists have come to suspect that the molecular constituents of Surflon S-111 and the thousands of other PFASs in global commerce pose hazards similar to those of PFOA. Regulatory agencies are attempting to address them collectively.⁷⁵ The EPA negotiated a voluntary phaseout of “long-chain PFASs,” a subclass thought to be most persistent and toxic; the FDA removed three such chemicals from its list of approved food-contact substances.⁷⁶ Yet these efforts, too, are built on molecular bureaucracy. Giving a chemical class legal and administrative meaning required the painstaking assembly of a corresponding molecule-by-molecule list—PFOA, Surflon S-111, and 219 other chemical substances, in the case of long-chain PFASs restricted from use in carpets or carpet-care products.⁷⁷ Furthermore, chemical classes have molecular borders. As long-chain PFASs have been phased out, they have been replaced by short-chain PFASs and other chemical analogs lying just outside the molecular bounds of the restricted class, such as the PFOA substitute “GenX” manufactured by DuPont spinoff Chemours. A group of environmental scientists published a consensus statement urging efforts to phase out all PFAS chemicals, leading to an exchange of statements with a fluorochemical trade group over what exactly

⁷⁵ Wang et al., “A Never-Ending Story”; “Occurrence and Use of Highly Fluorinated Substances.”

⁷⁶ Alissa Cordner, Lauren Richter, and Phil Brown, “Can Chemical Class Approaches Replace Chemical-by-Chemical Strategies? Lessons from Recent U.S. FDA Regulatory Action on Per- And Polyfluoroalkyl Substances,” *Environmental Science & Technology* 50 (2016): 12584–91.

⁷⁷ “Significant New Uses: Perfluoroalkyl Sulfonates and Long-Chain Perfluoroalkyl Carboxylate Chemical Substances,” US Federal Register of 22 October 2013, 78 FR 62443–62451.

this class of chemicals should comprise. The arguments in this exchange, addressing risk, benefit, and epistemology, stand apart from molecular bureaucracy.⁷⁸ So does the logic of industrial capitalism underlying the replacement of banned chemicals by substitutes that minimized disruptions to existing systems of production while remaining legally and politically defensible. But the criteria of similarity and difference according to which defensible but not disruptive substitutes could almost certainly be found, and the specific chemicals developed as substitutes, posing “intractable, potentially never-ending” environmental effects: these were molecular bureaucracy’s material consequences.

One can hardly treat the diversity of matter as an epiphenomenon of a database. That would be silly. Histories of environmental chemicals are shaped by materials, environments, power, and politics. Chemical databases and environmental regulations were and are shaped by such factors as well. But bureaucracy has a life of its own. Molecular identity, information coordination, and chemical holism form a collective framework for myriad efforts to control the political identity and environmental consequences of anthropogenic chemicals. They constitute a legal and administrative “body of chemical and biological data.” Molecular bureaucracy is an interface where law, administration, and politics meet empirical measurement and the material world. It is the game board on which the moves and countermoves of regulatory politics play out.

⁷⁸ Arlene Blum et al., “The Madrid Statement on Poly- and Perfluoroalkyl Substances (PFASs),” *Environmental Health Perspectives* 123 (2015): A107–11; Jessica S. Bowman, “Fluorotechnology Is Critical to Modern Life,” *Environmental Health Perspectives* 123 (2015): A112–A113.

Beyond Molecular Bureaucracy?

This essay has sketched the outlines of molecular bureaucracy, focusing on the US institutions in which it took shape. Understanding its scope and limits will require extending this analysis, in dialogue with scholarship on other aspects of environmental science, politics, and governance. Does global molecular bureaucracy derive primarily from these American origins or from convergent developments, and what alternatives has it foreclosed? What role has molecular bureaucracy played in the constitution of toxic sacrifice zones within politically disempowered communities, the global south, and the sea? What are the distinctive consequences of addressing metal pollutants according to their single-atom molecular identities (i.e. the chemical elements “lead,” “mercury,” and so on)? Which aspects of molecular bureaucracy are specific to environmental chemicals, and which are echoed in air pollution, climate politics, biodiversity preservation, agricultural biotechnology, and other domains of environmental regulation?

For now, I conclude with a few remarks on what activists and engaged scholars are trying to do about molecular bureaucracy, and how its history can help. The preponderance of these efforts defend, refine, and make use of molecular bureaucracy. Scholar-advocates are speaking out about threats to the reformed TSCA and the information systems that support it.⁷⁹ Adapting methods from computational genomics, scientists are seeking to interconnect molecule-by-molecule toxicity data into a holistic picture of the “exposome.”⁸⁰ Market-oriented organizations are developing lists of chemicals of concern like the long-

⁷⁹ Lindsey Dillon et al., “The Environmental Protection Agency in the Early Trump Administration: Prelude to Regulatory Capture,” *American Journal of Public Health* 108 (2018): S89–94.

⁸⁰ Christopher Paul Wild, “The Exposome: From Concept to Utility,” *International Journal of Epidemiology* 41 (2012): 24–32.

chain PFASs, as a basis for sustainable business practices and consumer empowerment.⁸¹ Scholars engaged in community-based participatory research are using molecular bureaucracy—“parasitizing the CAS Registry,” as one group puts it—to constitute open-source, community-based databases of information about toxicity.⁸² Social scientists call for improved interagency coordination and international data sharing—that is, for the continuation of the longstanding project of coordinating information about toxic hazards.⁸³ This study suggests that such efforts are well positioned to take advantage of myriad existing information resources and deep grooves of bureaucratic habit, but that there are limits to what can be achieved within the frame of molecular bureaucracy.

Others are engaged in the daunting task of working out scientific, political, and historiographic alternatives to the logic of molecular bureaucracy. To cite three promising examples: first, practitioners of “green chemistry” and “green engineering” are reconceiving safer chemicals research and development not just in terms of the structure and properties of end products but their entire life cycle, from starting materials to byproducts to disposal and degradation.⁸⁴ Second, a group of historians and sociologists advocates addressing environmental chemicals as residues: byproducts of irreversible processes, characterized by persistent neglect, by the capacity to slip across the boundaries of bodies and systems, by unpredictability, and by their strictly negative status of matter to be cleaned up. Residues, these authors emphasize, are joint projects of the unruliness of

⁸¹ Geiser, *Chemicals without Harm*.

⁸² Sara Ann Wylie, *Fractivism: Corporate Bodies and Chemical Bonds* (Durham: Duke University Press, 2018), 92–94 (quotation on 94); Scott Frickel and James R. Elliott, *Sites Unseen: Uncovering Hidden Hazards in American Cities* (New York: Russell Sage Foundation, 2018).

⁸³ Cordner, Richter, and Brown, “Chemical Class Approaches,” 12589.

⁸⁴ Paul T. Anastas and Julie B. Zimmerman, “Safer by Design,” *Green Chemistry* 18 (2016): 4324.

matter and of social practices that allocate value and attention.⁸⁵ Third, bringing Indigenous and feminist standpoints to community-based research, anthropologists including Elizabeth Hoover and Vanessa Agard-Jones have addressed environmental chemicals as relations through which humans are collectively, inextricably, and unequally entangled with industrial products.⁸⁶ Murphy argues that this conception of chemically-entangled bodies and ecologies, which she terms “alterlife,” calls for strategic engagement of chemistry and toxicology, working “with and against technoscience” while resisting its “epistemic habits,” to acknowledge chemical entanglements and their histories.⁸⁷ STS scholars Nicholas Shapiro, Nasser Zakariya, and Jody Roberts call for getting off the “data treadmill” and engaging grassroots perspectives that raise fundamental questions about environmental toxicity forgotten in the din of adversarial encounters involving toxicological information.⁸⁸

The history of molecular bureaucracy can enrich such efforts with the insight that the “technoscientific epistemic habit” of equating matter with molecules is largely a *bureaucratic* habit. Picking through the chemical sciences for research relatively easily dislodged from bureaucratic databases and legal definitions may be a promising strategy both for working “with and against technoscience” and for describing this tactic to collaborators in natural sciences and engineering. Conversely, escaping molecular bureaucracy means not taking its objects for granted. If “human thought and culture are

⁸⁵ Boudia et al., “Residues.”

⁸⁶ Vanessa Agard-Jones, “Bodies in the System,” *Small Axe* 17, no. 3 (2013): 182–192; Elizabeth Hoover, *The River Is in Us: Fighting Toxics in a Mohawk Community* (Minneapolis: University of Minnesota Press, 2017).

⁸⁷ Murphy, “Alterlife,” quotations on 495, 497.

⁸⁸ Nicholas Shapiro, Nasser Zakariya, and Jody Roberts, “A Wary Alliance: From Enumerating the Environment to Inviting Apprehension,” *Engaging Science, Technology, and Society* 3 (2017): 575–602.

intimately embedded in their bodies and the material environment,” as environmental historian Timothy LeCain has written, so too are the entities taken to constitute bodies and material environments—by natural scientists and especially by fellow-traveling humanists and social scientists—intimately embedded in human thought, culture, politics, and power, concretized in information systems and administrative procedures.⁸⁹ The history of molecular bureaucracy encourages the scholar of environmental chemicals to adopt the perspective of a “materialist who understands matter as the effect of tools, practices, and power,” as Murphy puts it.⁹⁰ Finally, the history of molecular bureaucracy offers a road map for engaged scholars interested in making alternative chemical ontologies into normative modes of knowledge and politics. Molecular bureaucracy gets things done, is entrenched, and appeals to many constituencies (even as it frustrates them). Those who wish to install a different approach to the regulatory politics of environmental chemicals should appreciate what has made molecular bureaucracy stick, and the practical limits of unsticking it. Bureaucracies have residues, too.

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Evan Hepler-Smith is a Core Fellow and Visiting Assistant Professor of History at Boston College. From 2016 to 2018, he was a postdoctoral fellow at the Harvard University Center for the Environment. His research addresses the intersecting histories of industrial chemistry, information technology, and environmental toxicity. He is currently completing a book on the role of information management in the making of modern chemistry and the global synthetic chemicals industry.

⁸⁹ LeCain, *The Matter of History*, 16.

⁹⁰ Murphy, *Sick Building Syndrome*, 177.