

URSULA KLEIN

INTRODUCTION: TOOLS AND MODES OF REPRESENTATION IN THE LABORATORY SCIENCES

Like most key epistemological concepts, "representation" has provoked both enthusiasm and skepticism. For many science study scholars and historians of science, the prospect of re-thinking a familiar epistemological category and opening it up to scrutiny has been an intriguing intellectual challenge.¹ In their studies the term "representation" means signification or reference without any simultaneous commitment to realism. By contrast, speech about "representation" in philosophical discourse often implies an investment in realism, in the belief that texts, pictures, and other sign systems correspond to autonomous objects in the world out there. As a result, studies on "representation" frequently are conceived of being informed by a "representational idiom" which casts scientific knowledge as something that "maps, mirrors, or corresponds to how the world really is."² "Representationalism" is another slogan which assigns "representation" to the metaphysics of realism, connected with the denial that the notion of "representation" has any useful role.³

Problems of realism, correspondence, and truth are not at stake in this volume. Contributors do not share a single epistemological perspective, but they all agree that representation or signification is an intrinsic element of laboratory sciences, which can be opened up to detailed empirical investigation just as previous scrutinies of experimental intervention were. The work of laboratory scientists consists to a considerable extent in purifying experimental marks, processing data, and producing and reading tables, graphs, diagrams, pictures, formulas, mathematical equations, 3-D models, texts and so on. "Tools and Modes of Representation in the Laboratory Sciences" is a loose frame for historical reconstructions and philosophical discussions of such representational practices. The volume tackles questions such as: How did scientific practitioners make sense of mathematical representations of theoretical entities? How much did their understanding depend on transformations of mathematical sign systems into diagrams, graphs or other iconic modes of representation? Are modes of representation conceptually essential or merely decorative features of scientific discourse? Why did experimental scientists implement theoretically loaded sign systems, such as chemical formulas, in their practical activities, and what were the functions of such sign systems in experimental practice?

The volume seeks to portray the endeavors and enormous efforts of scientists to construct working representations, be they the structural formula of a dye, the three-dimensional model of a protein, a table conveying relationships between chemical elements, diagrams depicting functional relationships of the genetic apparatus, or a lengthy text dealing with the molecular level of objects. It investigates contingent socio-historical conditions and material resources that contributed to representational

practices. The historical focus is on nineteenth-century and twentieth-century chemistry and biochemistry, as well as the intersections of these disciplines with other experimental cultures, such as crystallography, molecular biology, and molecular physics. The epistemological focus is twofold. First, on the intertwinement of denotation and labeling with historically, socially and culturally situated meaning; and second on the relationship between specific modes of representation and differentiation of meaning.

Nelson Goodman and others have argued that "representation of," or denotation, must be supplemented by "representation as" or meaning.⁴ A representation A of an entity B is not merely a denotation of it, but also creatively describes and classifies it as such-and-such. Representation, Goodman asserts, is not a matter of passive reporting, and "the object does not sit as a docile model with its attributes neatly separated and thrust out for us to admire and portray."⁵ Rather, representation involves organization, invention, and other kinds of activity. This view concords with approaches in epistemic sociology that seek to embed representation in local contexts of communicative activity. Michael Lynch, for example, asserts that understanding sign systems is a "variegated, and 'located,' communicational production," and that referential functions are "embedded in action."⁶ He relates this to Ludwig Wittgenstein's notion of language-game embedded in the performative context of a collectively shared "form of life." As David Bloor has observed, many of Wittgenstein's examples for language-games involve work and labor.⁷ On this view language-games are not merely social interactions that constitute self-reference but include interactions between humans and humans as well as between humans and things or other non-humans.⁸ The history of experimentation provides an arsenal of examples, both for the intrinsic connection of denotation and meaning and for the multifaceted ways they are entrenched in social and material actions.

As a rule, laboratory scientists investigate invisible objects – such as atoms, molecular structure, chemical reactions, gene expressions, electromagnetic waves and so on – which are accessible to experience only via their experimentally produced effects or marks. Unlike practice with ordinary objects in everyday life, the denotation and labeling of these invisible objects is performed without any direct ostension. Rather, it is tied to processing and interpreting the experimental marks of the invisible object, and to the application of sign systems, culturally impregnated with meaning, in that endeavor. With respect to experimentation most philosophers today agree that it is impossible to distinguish analytically between representational elements that are given to human experience and those elements that are culturally and socially constructed and self-referential. For these philosophers, the laboratory sciences make obvious that "representation of" and "representation as" always come together. Further, recent approaches to experimentation in the history, philosophy and sociology of science have paid attention to material culture, the mutual adjustment of its elements, and developmental processes. Their overall depiction of experimentation as a specific form of collective human action that has a certain "life of its own" and provides scientists with unexpected, surprising phenomena is at odds with the reduction of experimentally contextualized reference to social self-reference.⁹ A general conclusion that can be drawn from such studies is that the material target of experiments, its preparation and adjustment to instruments and apparatus, the material traces or data produced by human manipulations and physical interactions between the object of inquiry and the physical instruments, are as

constitutive of reference in laboratory sciences as cultural sign systems and their manipulation and superposition, collectively shared classifications and associated conceptual frameworks, and various forms of collective action and social institutions.

This raises the question of how much modes of representation, and specific types of sign systems mobilized to construct them, contribute to reference. Semioticians have argued that sign systems are not merely passive media for expressing preconceived ideas but actively contribute to meaning. Sign systems are culturally loaded with meaning stemming from previous practical applications and social traditions of applications. In new local contexts of application they not only transfer stabilized meaning but also can be used as active resources to add new significance and modify previous meaning. This view is supported by several analyses presented in this volume. Sign systems can be implemented like tools that are manipulated and superposed with other types of signs to forge new representations. The mode of representation, made possible by applying and manipulating specific types of representational tools, such as diagrammatic rather than mathematical representations, or Berzelian formulas rather than verbal language, contributes to meaning and forges fine-grained differentiations between scientists' concepts.

Taken together, the essays contained in this volume give us a multifaceted picture of the broad variety of modes of representation in nineteenth-century and twentieth-century laboratory sciences, of the way scientists juxtaposed and integrated various representations, and of their pragmatic use as tools in scientific and industrial practice. The resulting depiction rejects expectations that laboratory scientists might over time select those particular modes of representation which are generally regarded to be "rational," i.e. belonging to the logical type of sign systems. Moreover, it conveys a plethora of concrete ideas about how scientists implement signs systems in their activities as productive tools not only to achieve, but also to shape their representational goals.

The first series of articles is concerned with different types of chemical formulas and their various representational functions in chemical practices. Chemical formulas, introduced by Jacob Berzelius in 1813 and broadly accepted by the European chemical community in the late 1820s, are as emblematic of the laboratory science of chemistry as flasks, beakers, distillation columns and so on. These eminently chemical symbols, which today pervade not only chemistry, biochemistry, and molecular biology but even everyday life, are closely related to the working life of theoretical chemical concepts, first to the concept of scale-independent chemical portion and later to the concepts of atom, molecule, and atomic structure. *Alan Rocke's* essay provides a broad historical overview of the problems and approaches related to this issue in nineteenth-century European chemistry. Nineteenth-century chemical atomic theories have often been treated as a decontextualized set of ideas, concepts and hypothetical statements. Rocke instead portrays the various facets of "chemical atomism" as a network, "leaky as a fishnet," of physical principles and simplicity assumptions, sets of analytical data inscribed in the laboratory, and formulaic notations and tabulated systems of invariable combining weights, constructed on the drawing board and inserted in various ways into texts embodying atomistic hypotheses. Because atoms, in the sense of discrete portions or units of chemical elements and compounds, were both the intended

referents of chemical atomism and entirely beyond laboratory observation, it is not surprising that the issue of reference was constantly on the agenda of nineteenth-century European chemists and the subject of fierce debate. Rocke proposes to embed nineteenth-century chemists' "styles of theorization" into these controversies, as these were sustained by the shared goal of a pragmatic use of chemical atomic theory, the application of chemical formulas as paper tools, conventional standardization, and communication across systems.

The first type of chemical formulas, the quasi-algebraic formulas introduced by Jacob Berzelius in 1813, are the subject of *Ursula Klein's* essay. The essay, which connects semiotic analysis with contextualized historical investigations of the practical application of Berzelian formulas, suggests a new view of this sign system as productive "paper tools," rather than as a passive medium for expressing and illustrating already existing knowledge or beliefs. The term "paper tool" is introduced to emphasize the material, performative and generative aspects of sign systems in scientific practice. The historical focus is on the constitutive role played by chemical formulas in Berzelius' elaboration of a theory of "chemical portions" as an alternative to Dalton's atomic theory, and on the subsequent application of Berzelian formulas in organic chemistry as paper tools for constructing models of the constitution of organic substances and for creating new classifications.

Structural formulas, or graphical formulas as they were sometimes called, were introduced into chemistry in the late 1850s. This two-dimensional notation, which consisted of letters (or letters and circles) and lines, referred to "chemical structure," i.e. the order or succession in which individual atoms are chemically combined with each other. *Christopher Ritter* studies the introduction and further application of structural formulas as a process which was stimulated and advanced simultaneously by theoretical interests, laboratory practice, didactics, and techniques of visualizing. His paper pays renewed attention to an early achievement in establishing structural formulas, Alexander Crum Brown's 1861 M.D. thesis, arguing that it should be interpreted as a state of transition from type formulas to structural formulas, with a bridging hybrid formula that mediated the two notations. Crum Brown's new concept of "polar forces," Ritter argues, was stimulated by visual displays of his diagrammatic mode of representation.

Pierre Laszlo tells the story of structural formulas as a history of their textualization, de-textualization and re-textualization, along with analyses of conventions of writing. The iconic status of structural formulas depends on their relation to other sign systems, in particular to texts. Early structural formulas (1865–1905), Laszlo asserts, usually were aligned with texts and read as integral parts of texts. Chemists viewed them as a kind of condensed narration summarizing conclusions drawn from work in the laboratory which investigated chemical transformations. This function was stabilized by arbitrary conventions of writing and printing, or "formulaic orthography." The proper orientation of formulas on the printed page facilitated "pattern recognition" as a visual clue to the kind of chemical reaction and the identification of the denoted substances. According to Laszlo, only after 1905 did structural formulas assume iconic status, then depicting the geometry of molecules, and move into the blank spaces of the page to become re-textualized again in nascent computer chemistry after 1949.

The stereochemical formulas developed from structural formulas in the 1870s and 1880s were mainly the result of the integration of different areas of chemical

knowledge informed by theoretical considerations. Just like the multiple progeny of a single structural formula, stereochemical formulas often referred to chemical compounds which existed only on paper, in a fictional world. Yet explorations on paper, *Peter Ramberg* argues in his essay, were also responsible for spurring chemists to create a large number of new artificial compounds in the laboratory. Chemists used structural and stereochemical formulas as paper tools to construct predictions which corresponded with their theoretical assumptions and fitted their classificatory order of existing substances and reaction types. Analogies of formulas were a powerful way to forge these fits. Whether predicted compounds were actually synthesized in the laboratory, Ramberg emphasizes, also depended on chemists' craft-like skills and their ability to adjust gestural techniques to local experimental situations.

The paper by *Carsten Reinhardt* and *Anthony S. Travis* continues with the theme of chemical formulas, investigating the role played by constitutional and structural formulas in the industrial-academic context of dye fabrication. The partnership between the synthetic aniline dye industry and academic chemistry, established from the middle of the nineteenth century particularly in England and France, was entrenched by the common "language" of chemical formulas. Reinhardt and Travis argue that this partnership was not an unbalanced dependence of industry on academic research, but rather a mutual interaction in which industrial interests also stimulated academic research, including investigations for the development of useful products and those conducted to identify and classify pure dyes so that they could be represented by constitutional formulas (or "type formulas") and structural formulas.

The tool box of chemists, biochemists, crystallographers, and molecular biologists was enriched in late-nineteenth-century by another item that is no less productive and powerful than chemical formulas: physical, three-dimensional molecular models. Based on two case studies on the practical application of three-dimensional "space-filling models" – one on structural investigations of proteins by biochemist Hans Neurath, crystallographer William Astbury, and chemist Hugh Taylor in the 1930s and 1940s, the other on Linus Pauling and Robert Corey's use of especially developed space-filling models in connection with their discovery of the alpha-helix of polypeptide chains – *Eric Francoeur* argues that focusing on the material culture of representation yields novel insights into processes of scientific innovation. Used as substitutes for intractable calculations or as devices for exploring steric hindrance through touch, space-filling models became an important epistemic resource whose material properties contributed to the emergence of particular features of scientists' objects of study. For example, in his attempts to assemble a space-filling scale model of Astbury's alpha-keratin structure, Neurath realized that there was simply not enough room for all of the atoms and that steric hindrance made that model unlikely.

Today Linus Pauling is well-known as a master of a whole world of three-dimensional molecular models. In her essay, *Mary Jo Nye* investigates the question of the circumstances and concerns that led Pauling to complement his early paper tools of mathematical and structural chemistry with three-dimensional models. While Pauling was preoccupied with research on quantum chemistry in the late 1920s, his research interests after 1932 turned to biologically significant molecules as his university, Caltech, increasingly had come to depend on funds supporting a



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