Scientific Agency and the Conceptual Dynamics of Science

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The role of action, and especially the conditions of action, in scientific change and progress have received relatively little attention in philosophy of science. Yet certain kinds of important scientific change seem to be about the transformation of agency rather than the theory change philosophers have generally focused on. The conditions of agency determine what is and is not possible for an agent to do, and these possibilities are crucial to the production of scientific knowledge and to the course of scientific development. I argue that philosophical theories of scientific change and progress need to attend more closely to the dependence of theory development on the nature of scientific agency. This dependence is strikingly evident in the history of chemistry, where experimentation, rather than theorizing, has been the dominant activity. I propose what I call the Agency View of scientific progress that attempts to articulate changes at the level of agency with theory development.

Keywords: Instrumental Revolution; Agency; Scientific Change; Structure Determination; Technology; Progress; Mechanization; Labor

Contents

1 Introduction

In the study of scientific change, philosophers of science have traditionally focused on changes in scientific theories. Scientific knowledge is construed as propositional knowledge, and the aim of science is construed as the acquisition of knowledge in the form of systems of justified, true propositions about the world. Scientific change itself is understood largely in its discursive dimension, as resulting from the way accepted theories are related to new propositions generated by experiment and observation.[1]

In contrast, the role of action, and the conditions of action, in scientific change and progress have received relatively little attention in philosophy of science.[2] Yet certain kinds of important scientific change seem to be about the transformation of agency rather than the theory change philosophers have generally focused on. The conditions of agency determine what is and is not possible for an agent to do, and these possibilities are crucial to the production of scientific knowledge and to the course of scientific development. In this essay I argue that philosophical theories of scientific change and progress need to attend more closely to the dependence of change and progress on the nature of scientific agency, and I show that this dependence is especially evident in the history of chemistry, where experimentation, rather than theorizing, has been the dominant activity.

By 'agent' I mean an entity capable of purposive action, and by 'agency' the exercise of this capability. The agent's capabilities delimit a horizon of possible actions for the agent. By 'horizon' I mean that the capabilities simultaneously limit, but also make possible, actions for the agent. Thus a human agent is capable of engaging in a horizon of possible actions in virtue of his or her physical and mental capabilities. This horizon differs from that of other animals, in virtue of their different capabilities. Tools allow humans to expand their capabilities, and hence their horizon of possible actions. For example, whereas

[1] See Losee (2004) for a survey of philosophical theories of scientific change.
[2] Notable exceptions to this are Hacking (1983), Gooding (1990), and Chang (2011, 2012). Note that by invoking action, I intend any scientific work at all, not just experimentation. I will say more on this point in the conclusion.

I am incapable of constructing a lengthy text simply by exercising my memorial abilities, with writing instruments in hand I can write hundreds of pages.

Scientific theories also delimit a horizon of possibilities. For example, chemical structure theory prescribes all the possible arrangements in space that a group of atoms can assume. The theory thus prescribes ontic possibilities. But scientific theories can also entail certain possibilities for knowing the objects of those theories. For example, this same theory posits that the structures exist independently of chemical reactions. If that is the case, then under certain conditions it should be possible to know the structures independently of them. The theory entails an epistemic possibility.

When we relate the horizon of possibilities entailed by scientific theories to the agent's horizon of possible actions, we see that the realization of the possibilities inherent in the theory will depend on what it is possible for the agent to do. In the case of humans, the latter possibilities will depend on the instruments at their disposal. Even simple manual tools expand the horizon of possible actions beyond what humans are capable of in virtue of their native human abilities. In so doing, they facilitate the realization of the possibilities inherent in theories. To stay with the chemical example, the performance of chemical manipulations on substances by means of manual operations with balances, glassware and auxiliary equipment (Bunsen burners, spatulas, etc.) allowed chemists to explore the space of structural isomers defined by chemical structure theory.

Nevertheless, the expansion remains limited because actions by means of manual tools are still highly dependent on human abilities. *Machines*, on the other hand, introduce a qualitative shift by virtually emancipating the horizon of possible actions from the constraints imposed by native human abilities. Machines are not simply complex tools. At least since the Industrial Revolution, they have tended to replace and displace human labor, which can have significant effects on the potential for action and the potential for progress of the labor processes in which they are incorporated. These considerations suggest a novel epistemic function of machines: by emancipating the horizon of possible actions from the constraints imposed by native human abilities, they liberate the realization of the possibilities inherent in scientific theories from those same abilities.

My use of the word "emancipation" is intended to suggest that theory development may encounter obstacles at the level of agency. Among the more interesting of these sorts of obstacles are those that affect the basic routines and techniques of the science. Such obstacles do not merely impede the performance of a particular experiment, but affect the way the science is done in general. Their removal represents important inflection points in the development of the science.

Most philosophical treatments of scientific instruments treat them in terms of their role in experimentation, usually focusing on their characteristic outputs, such as measurements, models, and production of phenomena.[3] Davis Baird (2004) has noticed a modal role for spectrometers in the production of information: the spectrometer produces information by locating the specimen's signal in a field of possible values (e.g., a scale). I submit that a more general point can be made: machines are necessary to fully realize the possibilities inherent in scientific theories. It follows that the development of machine technology was a seminal event for the development of science, for once such a technology was available the possibilities inherent in scientific theories could be explored to a much greater extent than previously. It also follows that the mechanization of a science may signal a great leap forward in the ability of the science to develop its theories and study the entities posited by them.

Mechanization involves a transformation of the agent, from a human-tool agent to a human-machine agent. In science, such transformations may result in an adjustment of the agential horizon of the scientists to the ontic and epistemic horizon of the theories accepted by the agents. It also involves a transformation of agency, in that what the agent actually does changes. These transformations can be obscured by theory-centric views of science. Consider the following example from a 1965 textbook *Structures of Organic Molecules* on new methods of chemical analysis:

> Certainly much can be said in favor of the traditional approaches to organic chemistry … Chemical properties are emphasized in … these approaches. Historically these were the properties from which chemists deduced structure … This book takes an alternative approach to the subject, which is feasible at the present time … It begins with the assumption that the structures of organic molecules can be divorced entirely from chemical reactions. After all, the primary tools in the current routine identification of organic compounds are *theory* and *spectra*, and more often than not one can identify a given molecule without running any chemical reaction whatever.

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[3] Boon (2015), Rothbart & Slayden (1994).

Left out of the list of primary tools, however, are the machines that embody the theory and produce the spectra. But the alternative approach espoused by the authors presupposes mechanization, since prior to mechanization the last two propositions would have been false (this will become evident in the following sections).

The study of the transformation of agency through mechanization requires a different mode of analysis than the study of the sequence of scientific theories. In particular, the *epistemic roles* of the agents and their instruments must be examined historically. By "epistemic role," I intend the activities carried out by the agent insofar as they contribute to the acquisition of knowledge. Thus, explaining, detecting, manipulating, causing, understanding, and interpreting are scientific activities (among many others, of course), and it is the role of the agents and instruments in scientific work to carry them out.[4]

My theses based on these considerations are as follows:

1. certain kinds of important scientific change consist of the transformation of scientific agency
2. the transformation makes possible the realization of possibilities inherent in scientific theories
3. changes in the epistemic roles of the agents and their instruments explain why certain theoretical possibilities, which could not be realized before the changes, were realizable after the changes.

I will call the combination of these theses the "Agency View" of scientific change. I will demonstrate them for the case of what has been called the Instrumental Revolution in chemistry, which saw the birth of the new methods alluded to above. I argue that changes in the epistemic roles of chemists and their instruments explain a significant change in the conception of chemical structure and bonding, both why the change happened when it did and its content.

The paper is organized as follows. I describe chemical structure analysis before and after the Instrumental Revolution in section 2. For space reasons I have left the description

[4] Chang (2011) calls such activities "epistemic activities," which according to him are articulated together as coherent "systems of practice."

impressionistic, and I refer the reader to my more detailed account elsewhere.[5] In section 3, I provide evidence that the Instrumental Revolution involved a conscious effort to restructure chemists' agency around machines, largely by applying science and technology to restructure the labor process around what I call "strategic functions." In order to have a model to guide the analysis, I will compare this case to another sort of transformation of agency, the mechanization of ordinary material labor. In section 4, I argue that these changes at the level of the labor process allowed certain important possibilities of chemical structure theory to be realized. I offer concluding remarks on the Agency View and its relation to a few theories of scientific agency and activity in section 5.

2 Structure Determination Before and After the Instrumental Revolution

Chemists call the activity by which they produce claims about the structures of molecules *structure determination* or *elucidation*. The "Instrumental Revolution," as it was dubbed by the chemist-historians Dean Stanley Tarbell and Ann Tracy Tarbell,[6] refers to a transitional period lasting roughly from the 1940s through the 1960s during which powerful new sources of evidence for molecular structure were introduced in the form of spectroscopic instrumentation. The United States was the epicenter of these changes. Techniques such as nuclear magnetic resonance spectroscopy, mass spectrometry, infrared and ultraviolet spectroscopy, gradually displaced the chemical reaction as the principal source of evidence for structure. These techniques permitted a massive increase in the productivity of chemical analysis work and also provided access to new kinds of information on molecular structure and dynamics. Not only did the techniques change, but so did the skills needed to employ them. Cheap glassware was replaced by expensive machinery, and wet chemical skills were replaced by machine operation skills.

[5] Borg, "On the application of science to science itself: chemistry, instruments and the scientific labor process," under review.

[6] Tarbell & Tarbell (1986), ch. 21. The nature of the episode does not lend itself to precise dating. Some important innovations and new techniques started to be developed as early as the 1910s (e.g., X-ray crystallography) whereas other important developments (like multi-dimensional NMR spectroscopy) only reached fruition in the 1970s and 1980s. Nevertheless, most historians locate the high tide of change in the middle decades of the 20th century. The historiographical debate over how to interpret the Instrumental Revolution is largely contained in Morris (2002), a volume of essays on the period by historians and philosophers of science, and Reinhardt (2006), ch. 1.

In general, the goal of structure determination is to determine the connections between atoms in a molecule, and often the spatial properties of the molecule as well. The chemical structure theory established in the late 19th century provided rules for determining the possible connections and spatial arrangements of a group of atoms. With the acceptance of this theory, chemists could turn the observations furnished by chemical reactions into evidence for molecular structure.[7] Structure determination became one of the major activities of the field.

The classical era of structure determination stretched from the 1860s to the 1950s, during which time chemists determined the structures of many complex natural products, including dyes, pigments, alkaloids, vitamins and hormones. The determination of complex structures using chemical "wet" methods was extremely time-consuming, often taking decades and sometimes even leading to the award of Nobel prizes.[8] A famous example is strychnine, which was isolated in 1815 but whose structure was not definitively established until 1948 despite intensive efforts on the problem: at least 245 papers were contributed to solving it between 1891 and 1950, and one of the principals in the field, Robert Robinson, was even awarded a Nobel Prize for his "investigations in plant products of biological importance."[9]

Classical chemistry was heavily dependent on the performance of manual work by the chemist.[10] It was also conservative in its methods, as this quote from the chemist-turned-historian David Knight illustrates well:

> The chemistry that I learned in school and at university in the 1950s was essentially nineteenth-century … To someone with my training, the history of chemistry in its golden age … was accessible. It was no surprise that Jacob Berzelius [1779-1848] should have written a whole book about using the blowpipe, or Michael Faraday [1791-1867] a stout volume on *Chemical Manipulation* [1827] (still full of useful tips to my generation, on weighing, getting ground-glass stoppers out of bottles, and distilling); or that William

[7] Sidgwick (1936) offers a clear and concise description of the theory and its development up to 1936. See Brock (1993), ch. 7 for a treatment of the rise of structure theory.
[8] A list is provided in Morris & Travis (2002), p. 60.
[9] "The Nobel Prize in Chemistry 1947". Nobelprize.org. Nobel Media AB 2014. Web. http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1947/. (Accessed 24 July, 2015). See Slater (2001) for an account of the strychnine research.
[10] Modern chemistry continues to be dependent on manual chemical manipulations, though the field of application has changed (e.g., to synthesis) and labware is largely purchased rather than made in-house.

> Ramsay [1852-1916] prided himself on his glassblowing … Physicists might look upon them as upgraded cooks; but chemists knew that they had learned a craft the hard way. They did not work with black boxes but with the transparency of glassware. Buying in apparatus was time-saving but not essential, and the really good chemist could be his own technician … Chemists also perceived the danger that an expensive toy … will be played with in time that, with more thought and less gadgetry, might be used for real discovery.[11]

A typical lab of the sort described by Knight is shown in Figure 1a.

In contrast with these 19th-century methods, the Instrumental Revolution ushered in new techniques based on physics, notably quantum mechanics. For example, nuclear magnetic resonance (NMR), one of the most powerful techniques of structure determination to emerge from this period, is the study of the properties of molecules containing magnetic nuclei. A magnetic field is applied and the frequencies at which the nuclei come into resonance with an oscillating electromagnetic field are observed. These frequencies depend on the chemical environment of the nuclei, and so the characteristic frequencies absorbed by a molecule provide evidence for its structure. The technique is of great importance for the structural analysis of organic molecules, like proteins, which contain magnetic ^{1}H and ^{13}C nuclei. A schematic of an NMR spectrometer is shown in Figure 1b. At the core of the instrument is a superconducting magnet, into which the probe containing the sample is inserted. Most of the apparatus is devoted to the generation, transmission and processing of a signal. The whole process is controlled by a device known as the pulse programmer ((4) in the diagram). The human operator types instructions at the computer, which are then loaded into the pulse programmer and executed from there. The operator also gives instructions for displaying, plotting and analyzing the data for structural information.

[11] Knight (2002), pp. 87-90; cf. Tarbell & Tarbell (1986), p. 335. Knight's comment about apparatus agrees with Jackson's (2015b) claim that "chemistry's move into home blown hollow glassware around 1830 … made it possible for chemists to work independently of professional instrument makers" (p. 189).

(a)

(b)

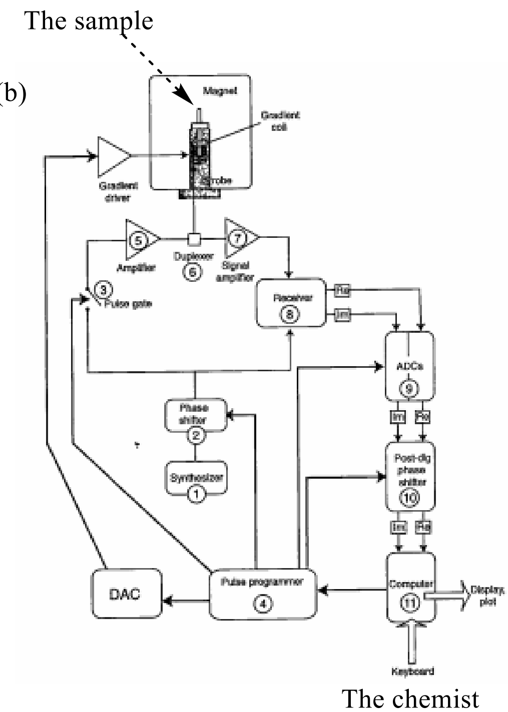

Figure 1.(a) A traditional chemistry lab in the 1940s of the sort described by Knight. Source: Morris (2015), p. 262. (b) The scene of the "crime:" a schematic overview of a pulsed-field NMR spectrometer. Source: Levitt (2008, p. 81).

As the schematic suggests, the spectrometer is a very complex combination of scientific principles and technology, drawing on a variety of fields including physics, electronics, computer science and mathematics.

These instruments were based on science and technology with which chemists were largely unfamiliar. They were also very expensive. Nevertheless, there was a significant pay-off for using them. Structure determination became much more efficient, freeing up the chemists' time for other work, such as synthesis or chemical applications in biology. Moreover, more complex targets could be tackled, for example biological macromolecules. The pay-off is evident in the case of strychnine mentioned above. Whereas over 245 papers were contributed over 60 years towards solving strychnine chemically,[12] only 6 were required over 5 years for the independent solution of the X-ray structure (Figure 2).[13]

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[12] Huisgen (1950).

[13] See the primary sources cited in Slater (2001), footnote 78.

(a)

(b)

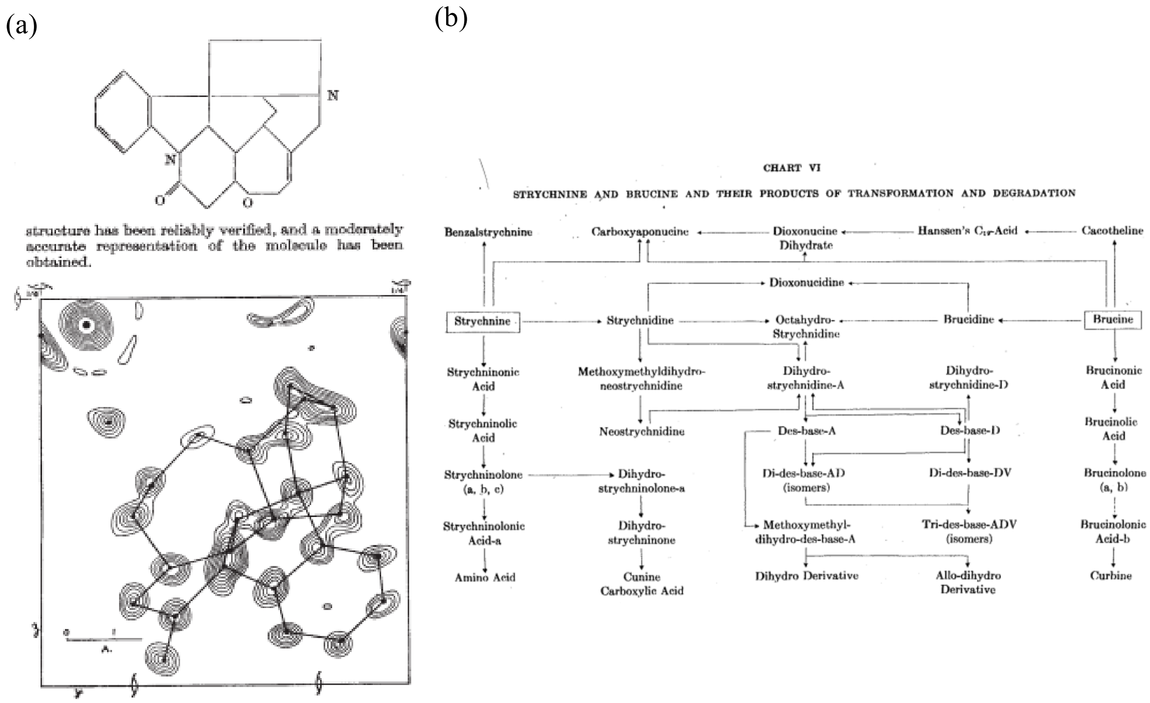

Figure 2. (a) These diagrams are from one of the first reports on the crystal structure of strychnine. The top diagram is a two-dimensional representation of strychnine. The bottom diagram is a contour map of the electron density on which a projection of the structure has been superimposed. Source: Robertson & Beevers (1950), p. 690. (b) The network of chemical transformations observed in the classical determination of the structure of strychnine and the closely related brucine. Source: Holmes (1950), p. 419.

This pay-off was accompanied by a significant change in the way structure determination was conducted. Whereas skills of chemical manipulation lay at the center of the classical methods, the new methods were centered on the interaction of machines with chemical samples.

In classical chemistry, the chemist would develop evidence for the structure of a substance by carrying out a set of manipulations on the latter. The means he employed were chemical reagents, glassware, balances, and auxiliary tools like heating sources, stirrers, stills, and pumps. By these means, the chemist would set chemical processes in train by means of various manual operations (weighing, adding, dissolving, heating, filtering, washing, drying, purifying, etc.). A chemist could identify the structure of an unknown by running it through a series of such processes designed to identify the various functional groups and their location in the carbon skeleton. This process was called "chemical degradation" because the reactions transformed the target into different, usually simpler compounds. The success of chemical research was heavily dependent on manipulative skills, as noted by Faraday in 1827.[14] The chemist would then interpret the results in terms of hypothesized structures. For example, chemists might accept such a hypothesis on the grounds that it best explained the network of chemical reactions obsevred for the substance (Figure 2b).[15] The interpretation of the results was often quite involved, requiring considerable chemical knowledge together with acumen for piecing together the results of reactions in terms of a structure.[16]

How do chemists use physical methods to obtain evidence for structure? Rothbart and Slayden (1994) provide an abstract description of spectrometers as "complex systems of detecting, transforming and processing information from an input event, typically an instrument/specimen interface, to some output event, typically a readout of information."[17] In spectroscopy the input event is the absorption or emission of electromagnetic radiation by molecules. Their response to the radiation generates a signal that carries information about the structure. The signal is transmitted by a "complex causal sequence of physical events from the specimen/instrument interaction to the readout."[18] The readout generally consists either of a spectrum or table representing the information in the signal (Figure 3) or, in the case of X-ray crystallography, a map of the specimen's electron density (Figure 2a). In modern chemistry, structures are determined by inserting an isolated sample into such systems. The chemist, who is generally not a designer or specialist of the instrument, has the roles of operating the instrument and interpreting the data. The role of her chemical laboratory skills is limited to sample preparation.

[14] Faraday (1827), iii.
[15] Hoffmann (2018) reviews several examples of classical structure determination. For an extended case study, see Slater (2001). Sir Robert Robinson has many examples in his (1976) autobiography. The textbooks by Mulliken (1904) and Shriner, Fuson & Curtin (1956, 3rd ed.) provide a systematic overview of classical methods.
[16] As attested in comments by veterans like R. B. Woodward (1963), Max Tishler (1983), and A. J. Birch (1995) (Woodward, 1963, p. 248; Tishler, 1983, p. 12; Birch, 1995, p. 22 and pp. 56-57). Textbooks from the mid-20th century contrasted the intellectual complexity of classical structure determination, which they sometimes compared to solving a jig-saw puzzle, to the simplicity of the new methods. See, for example, Wheland (1949), p. 127 and Allinger & Allinger (1965), p. 36.
[17] Rothbart & Slayden (1994), p. 29.
[18] Rothbart & Slayden (1994), p. 37.

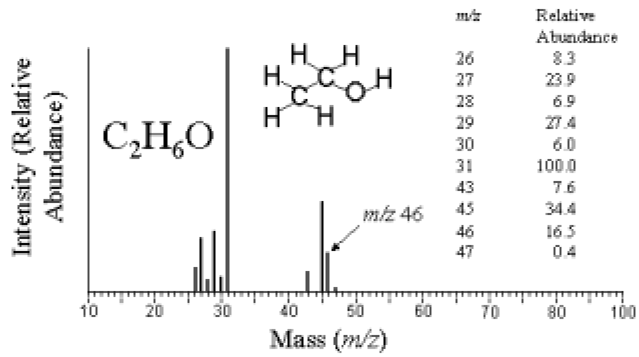

Figure 3. Partial mass spectrum of ethanol. The series of lines of varying intensity are referred to as the 'spectrum.' Their values and intensities are presented in tabular form in the inset. Source: Grayson (2004), p. 191.

If the basis of classical structure determination was the chemist's set of chemical laboratory skills together with his knowledge of chemical substances and their reactions, the basis of modern structure determination is the combination and adaptation of natural systems for the purpose of generating a signal that carries information about the specimen's structure. The decisive factor is not the skill of the chemist but whether this orchestration of systems is such as to produce a reliable signal.

The new methods did not dispense with the need for skill and know-how, however. Even in routine use, one must choose a solvent, the kinds of experiment to use, and interpret the spectrum, though in routine cases these operations are fairly standard. There was also an important element of continuity, in that the thing ultimately produced was a structural representation of a compound (as in Figure 2a), and this basically did not change. The Instrumental Revolution brought about a drastic change in how it was produced, however, involving a transition from a human-centered process to a machine-centered process.

3 Restructuring the chemist's agency

The restructuring of chemists' agency around machines was made possible by the application of prior scientific and technological knowledge. In this respect, it was similar to previous episodes of mechanization in economic production. Indeed, the economic growth theorist Simon Kuznets claimed that "the epochal innovation that distinguishes the modern economic epoch is the extended application of science to problems of economic production."[19] One question this claim raises is what makes the extended application of science to production possible?

Marxist analyses of the Industrial Revolution provide interesting insights into this question. An obvious answer is the growth of scientific knowledge. But as economic historian Nathan Rosenberg noted in his 1981 study of Marx's ideas on technology, the growth of science is not a sufficient condition for the application of scientific knowledge to the production process.[20] To believe that it is to ignore the mediating role of technology in the production process. Technology, in the form of the instruments of labor, mediates the process of transforming the object of labor and hence of realizing the producer's purposes. But

> not all technologies will permit, or will permit in equal degrees, the *application* of scientific knowledge to the productive sphere … It was one of Marx's most important accomplishments to have posed precisely this question: What are the characteristics of technologies which make it possible to apply scientific knowledge to the productive sphere?[21]

Science offers possibilities for enhancing the productivity of labor. The realization of these possibilities depends, however, on how the agents of production assign functions to people and things in the labor process. The distribution of those functions has a determining effect on the technological progress of production. In *Capital*, Marx analyzes two different ways of distributing those functions, what he calls "manufacture" (*Manufaktur)*, the predominant mode of capitalist production from the mid-16th century to the last third of the 18th,[22] and what he calls "large-scale industry" (*die große Industrie*), the mode of production that succeeded it. Manufacture was based on a division of labor between specialized workers wielding manual implements, an arrangement Marx calls the "subjective principle" of the division of labor in manufacture.[23] This "principle" encountered the limitation that

[19] Kuznets (1966), p. 9.
[20] Rosenberg (1981), p. 15.
[21] Rosenberg (1981), p. 15.
[22] Marx (1976), p. 455.
[23] Marx (1976), p. 501.

> Although … the manufacturing system achieved a growth of productivity through the exploitation of a new and more extensive division of labor, a rigid ceiling to the growth of productivity continued to be imposed by limitations of human strength, speed and accuracy … Science … cannot be incorporated into technologies dominated by large-scale human interventions.[24]

How was this problem solved? By the use of machines, of course, for "machinery may be relied upon to behave in accordance with scientifically established physical relationships."[25] The worker's skills can now be replaced by natural forces, thereby lifting the barrier to innovation posed by the limited abilities of human workers. Doing so permits the continual and free development of production by the "conscious application" of "the whole range of the natural sciences."[26] Innovation in production is all the more accelerated by the fact that science and technology develop synergistically, with advances in the former making possible breakthroughs in the latter, and vice-versa.[27]

It may seem that the causality implied in the last paragraph is the wrong way around. Wasn't it the application of science and technology that made possible the emancipation from native human abilites? But key to Marx's analysis of industrialization is the idea that the labor process has a structure involving functional relationships between the worker, the instruments and the object of labor. For him, the key step in the Industrial Revolution was the transfer of the tool-bearing function from workers to mechanical frameworks that could manipulate the tools. Though this move obviously depended on prior knowledge, it permitted much greater application of science and technology by allowing modifications of the tool-bearing mechanism as well as connections with other kinds of machinery, like engines. In general, the first steps in a process of mechanization may be fairly crude, as the potential for applying science and technology to it is only realized gradually.[28]

My suggestion, based on the foregoing, is that labor processes contain what I will call 'strategic functions.' What makes a function "strategic" is that its modification makes possible a pathway of transformations that might not be accessible from other starting-points. A relatively simple example is the development of the water frame. In Europe, up

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[24] Rosenberg (1981), p. 16.
[25] Rosenberg (1981), p. 16.
[26] Marx (1976), pp. 590, 616-617.
[27] Marx (1976), pp. 505, 508-509.
[28] Marx (1976), p. 505n18.

to about 1300 AD, fibers were spun into yarn by means of hand spindles. A single worker could manipulate one spindle at a time. In the late Middle Ages, the spinning wheel came into use. Here the spindle was mounted on a post and set in motion by using hand or foot to drive a large wheel attached to the spindle by a pulley. The drawing and twisting of the fiber was done by hand as the spindle rotated. Hargreaves' invention of the spinning jenny in 1764 made it possible to operate dozens of spindles simultaneously, because both the spindles and the fiber were now manipulated by a mechanical apparatus that was not limited by the number of arms in a human body. The mechanism itself was still driven by human force, however. Arkwright's water frame of 1769 was based on the same principle of mechanical spindle manipulation, but exploited the fact that human motive power had been made dispensable by the transfer of the spindle to a mechanism. The frame was now driven by a shaft that allowed it to be connected to a water wheel, thus allowing water power to be harnessed. Not only did this improve the productivity of the individual machine, but it allowed many machines to be connected by a transmission mechanism and so powered simultaneously by the same wheel, which further increased productivity.[29]

In this example, manipulation of the spindle played the role of strategic function. It was strategic because control over the tool had to be changed before water power could be exploited. The sequence could not have started with the application of water power, since the human arm is not easily detachable from its owner. This priority does not exclude that the two changes could occur simultaneously, in the same invention, say. The priority is logical, not temporal.

The transformation of a strategic function can make it more feasible to apply science and technology to the labor process. For example, the application of theories of heat and work to production, say in the form of the steam-engine, is made possible by the mechanization of tool manipulation. In this section, I will argue that *detection* played the role of a strategic function in chemical analytical instrumentation.

Importantly, these changes at the level of the labor process have cognitive counterparts. The "subjective principle" of manufacture involved, at the cognitive level, the assumption that however the production process was to be organized, each partial process carried out within it was to be done manually. The successor principle, which Marx sometimes calls

[29] Hills (1990), pp. 808-830; Usher (1954), ch. XI, section VI.

the “principle of machine production,” cognitively involved the discarding of this assumption. The “principle of machine production” does not refer merely to production by means of mechanical devices, but involves a problem-solving approach that analyzes production processes into their constitutive phases and draws on the entire store of scientific and technological knowledge in order to solve the problems of each phase and in order to connect the phases together. Thus, the ultimate import of the transfer of the tool-bearing function is that it paved the way for a much broader change in how problems of production were conceived and solved. This new way of thinking about production led in turn to further changes in economic production, which went far beyond the mere transfer of tools from one kind of bearer to another.

In short, what I take from the Marxist analysis of the Industrial Revolution are the following ideas. First, that the degree in which the technologies used in a particular production process are dependent on native human abilities affects the possibility of applying scientific knowledge to it. Second, that this degree of dependence is reflected in the problem-solving approaches used to address problems of production. Third, that labor processes contain “strategic functions” the transformation of which makes possible a pathway of transformations that might not be accessible from other starting-points. In some cases, the pathway of transformations may involve the extensive application of scientific and technological knowledge.

I will now provide evidence that a similar way of thinking, which one might call a “principle of machine production of data,” was influential in the Instrumental Revolution. Scientists involved in the Instrumental Revolution were animated by a new way of thinking about data production, one that consciously draws on scientific and technological knowledge as a whole rather than on the specific discipline in which the data is sought.

For example, James Feeney, co-author of a textbook on NMR, has periodized the progress of NMR in terms of alternating phases of science-driven and technology-driven development. The scientific discoveries underlying the method opened horizons for its application to structural analysis, but the technical requirements of the spectrometer entailed that “the full development of the method also relied on borrowing technology already being used successfully in other forms of spectroscopy and measurement.”[30] The

[30] Feeney (1999), pp. 206-207.

potential for applying NMR to structural problems other than very small molecules was not realized until improvements in the electronics and the magnet, the introduction of Fourier transform algorithms, improvements in computation, and yet other developments had come about.

Texts from the period of the Instrumental Revolution display the principle that analytical problems are to be solved by the replacement of human manipulations by the conscious application of science and technology. Analytical chemistry texts are particularly explicit on this point, perhaps because analytical chemistry became more directly concerned with the design of instrumentation than organic chemistry. For example, a report on the 1960 Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy states that the new instruments showcased that year all have in common that "[t]hey eliminate the human element, either partly or almost wholly."[31] Scientific texts also display the principle at work.[32] The physicist Paul Klopsteg called for the establishment of "instrumentology laboratories" the goal of which was to systematically apply science to the solution of problems across the natural sciences.[33] Klopsteg emphasized the comprehensive character of modern instrumentation. The disciplines he thought should be represented in these laboratories included physics, chemistry, mathematics, materials science, meteorology, geophysics, thermodynamics, acoustics, various kinds of spectroscopy, optics, and electronics. A 1958 review of the new instrumentation by the physical chemist S. Z. Lewin of NYU also emphasizes their eclectic character. Lewin examined trends in analytical instrumentation before and after World War II. He identified a "common feature" distinguishing post-war devices from pre-war, namely that

> [t]hese devices have been created by the conscious application of the principles of a relatively newly recognized discipline—the science of instrumentation—to the chemical need that was to be satisfied. The science of instrumentation is a hybrid field, drawing its content from optics, electronics, mechanics, circuit theory, computer theory, psychology,

[31] *Chemical and Engineering News* (1960), p. 106.
[32] Though space does not permit discussing these texts, the views of Heyrovský & Shikata (1925), Müller (1941), Ewing (1976), or Shoolery (1995) could be adduced as further evidence.
[33] Klopsteg (1945).

> and all those aspects of physics and chemistry that treat the interactions of radiant energy and electric or magnetic fields with matter.[34]

For Lewin, the "science of instrumentation" is not just a discipline dedicated to instrument-making, but an approach to "chemical needs" that is consciously eclectic.

Lewin's review is also noteworthy in that it suggests an explanation of the new instrumentation's origin. According to Lewin, every modern analytical instrument is composed of four fundamental components: a "transducer, or detector," an amplifier, a computer and an output. He likens the detector to "the eyes, ears, and nose of the instrument" and credits modern electronic detectors of radiation with greatly increasing the range of spectrometers, going so far as to claim that "their utilization in place of the photographic plate has been *directly responsible* for the current vigorous flowering of the fields of microwave, infrared, near-infrared, Raman, visible, ultraviolet and x-ray spectrometry."[35]

Lewin's assessment of the sources of progress suggests that the function of detection may have played a role analogous to that of the tool-bearing function in Marx's analysis. The key change, according to Lewin, was the switch from the detection of a chemical or physical property by exposure of a photographic plate to it, to the use of electronic detectors. According to Lewin, the photographic plate was the characteristic detector of pre-World War II analytical instrumentation. Lewin emphasizes the laboriousness of photographic plate detection:

> Compare, for example, the ultraviolet absorption spectra obtainable by means of photographic instrumentation commonly used in the 1930's with that provided by a modern recording spectrophotometer … With the older type of equipment several exposures of a photographic plate had to be made at different slit settings; the plate had then to be developed, dried, and microdensitometered; the results had to be compared with more or less laboriously achieved calibration data for the photographic emulsion; finally an absorption spectrum could be computed and plotted. The entire process required one to two days.

[34] Lewin (1958), p. 21A.
[35] Lewin (1958), p. 20A. My emphasis.

In contrast, with the use of the recording spectrophotometer "a pen moving across a paper chart automatically plots a finished absorption spectrum in a matter of minutes." This gain in time is made possible by the use of an electronic detector, in this case a photocell, which converts the incoming light from the sample into an electrical signal that can then power the recording device (what Lewin calls the output). The switch from the photographic plate to the photocell allowed the detector to be electronically connected to the output, which then allowed the recording of the signal to be automated. The signal generated at the detector may not be strong enough to power the output by itself, but since the detector is electronic it can be connected to an amplifier, which increases the signal to a usable level. Moreover, the signal may not be in a form suitable for providing the desired information at the output, and so connection with a computer is needed to transform the primary signal into the appropriate form. Depending on the output needed, the computer will be used to convert a current into a voltage, a direct current into an alternating current or vice-versa, modify the wave form of the signal, change the frequency, digitize the signal, etc.[36]

Lewin credits the combination of electronic detectors and amplifiers with bringing about significant scientific progress:

> The greater sensitivity, linearity, and reproducibility of electronic detectors and amplifiers, compared to such "classical" components of instruments as the human eye, photographic plate, and light-beam galvanometer, have now made it possible to sense, and to measure accurately, a vast array of substances for which no specific analytical method had previously been available, and at concentrations ranging from the pure substance down to 10^{-8} to 10^{-10} *M* and even less in favorable cases.[37]

Throughout his two-part review, Lewin emphasizes the scientific pay-offs, in terms of accuracy, sensitivity, resolution and range of application, that were made possible by the use of electronic detectors and their combination with other kinds of equipment.[38]

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[36] Lewin (1958), p. 22A (digitization is my example).
[37] Lewin (1958), p. 20A.
[38] Lewin's emphasis on the importance of the transition from photographic to electronic detection is corroborated by Hardy (1938), wherein the history of the first recording spectrophotometer (invented by the author) is described, and by the historians Morris & Eklund (1997), p. 559, and Thackray & Myers (2000), pp. 149-151.

For further corroboration of Lewin's claims, I will briefly discuss the strategic role of detection in mass spectrometry. In mass spectrometry, the components of a sample are ionized and then separated by various arrangements of electric and magnetic fields. The mass-to-charge ratio of each kind of ion is measured (Figure 3), and this information allows the components of the sample to be identified. Prior to the 1940s, the photographic plate was the most common method of detection. Starting in the 1940s, the photographic plate tended to be replaced by electronic detectors. As recounted in Grayson (2004), this seemingly unexciting modification eventually enabled the development of computerized systems capable of generating several hundred spectra per half hour, which by the 1990s could be compared via library search algorithms to libraries containing hundreds of thousands of reference spectra. In contrast, only a few spectra per week could be prepared and processed using the photographic method.

In summary, I have provided grounds for thinking that intervention on the strategic function of detection played an important role in the Instrumental Revolution. The intervention involved an evolution from processes in which humans were heavily involved in data production (e.g., the production and processing of photographic plates) to ones in which data production was increasingly automated. This evolution made possible the black-boxing of the instruments and hence their use for purposes of routine structure determination by organic chemists. Once the new methods were adopted by organic chemists, they supplanted the previous approach of solving chemical analysis problems largely through chemical methods, which also required heavy human involvement in data production. The progress made possible by the intervention required an eclectic approach to methods development in chemistry, one that drew on advances in diverse fields of science and technology in contrast to relying on the resources of a single discipline. This approach required dedicated instrument-makers, and the final users became for the most part non-specialists in their own instruments.

4 Realizing the possibilities of structure theory

In the introduction, I claimed that the transformation of agency makes possible the realization of possibilities inherent in scientific theories. How did this play out in the Instrumental Revolution? Let us consider again the passage from the 1965 textbook quoted in the introduction. Note the modality of the penultimate sentence: it claims that it is possible to divorce structure from reactivity. The claim seems to be open to two interpretations, ontological and epistemological. Ontological: the structures exist independently of chemical reactions. They do not simply summarize chemical reaction data. Epistemological: it is possible to know the structures independently of chemical reactions. This point is the focus of the last sentence, which further claims that it is *routinely* possible to know the structures this way. The two interpretations are compatible, and indeed the epistemological interpretation presupposes the ontological one, for only if the structures exist independently of chemical reactions is it possible to know the structures independently of them.

Under certain conditions, the independent existence could be part of a sufficient condition for the possibility of knowing them. Basic conditions were (i) that non-chemical data be available and (ii) that it be available in sufficient quantities to completely replace chemical reactions. Condition (i) was fulfilled by the nature of the new techniques, which were all based on the same basic principle: A substance is to be subjected to some energy probe and its response recorded. A single experiment yields all of a substance's responses to the probe. Thus in addition to X-ray crystallography and infrared spectroscopy, of the other techniques that came into common use at the time, ultraviolet spectroscopy records the response to ultraviolet light, NMR to radiofrequency radiation in the presence of a magnetic field, and mass spectrometry to bombardment by an electron beam of a definite energy. Condition (ii) was fulfilled by the informational yield of the individual techniques together with the fact that it was possible to develop a variety of such techniques, the combined data of which could solve most structural problems.

Before the Instrumental Revolution, these conditions did not exist. The revolution brought them into existence. As a result, the possibility of independent identification inherent in structure theory could be realized. Moreover, these conditions were brought about through the transformation of the agent involved from, put crudely, human scientists manipulating balances and glassware to human scientists operating complicated machinery supported by an extensive division of labor.

At this point, one might object that it was the reconceptualization of chemical structure in terms of quantum mechanics and spectroscopic properties that drove change in this episode, not mechanization. This objection ignores the historical development of the new methods. The realization of methods based on quantum mechanics required the transformation of labor. Each technique is indeed based on a physical phenomenon. But the latter was generally useless for other than the physicists interested in the phenomenon itself until the changes described in sections 2 and 3 took place. Mechanization was required to develop methods that had the speed, data storage capacity and control needed to produce data informative enough to replace chemical data. Black-boxing, an empirical approach to data interpretation,[39] and a new division of labor were other elements required to persuade organic chemists to abandon their traditional methods.

But the new instruments did more than realize the possibility of studying structure independently of reactivity. They also allowed an important theoretical lacuna to be filled, namely the question of how chemical bonds are realized. The classical structure theory developed by Kekulé and others in the 19th century made no assumptions about the mechanism of bonding. Bonds had what Hendry (2010) calls a “theoretical role” of providing links in the topological structure of molecules and constraining the spatial arrangements of atoms within them (thereby providing a foundation for stereochemistry). The question of how bonds are physically realized was left to empirical and theoretical investigations to answer. In his Presidential Address to the Chemical Society of London of 1936, the chemist Neville Sidgwick commented on the theoretical impact of the emerging new methods in these terms:

> [O]ur knowledge of the meaning of these structures has developed, especially in the last 20 years, to an enormous extent. We have applied to their investigation a whole series of physical methods, based on the examination of the absorption spectra in the infra-red, the visible, and the ultra-violet, and of the Raman spectra … To Kekulé the links had no properties beyond that of linking; but we now know their lengths, their heats of formation, their resistance to deformation, and the electrostatic disturbance which they involve. Throughout all this work the starting point has always been the structural formula in the ordinary organic sense. There is no better example of the effect of new discoveries in giving new meaning to a theory while they leave the truth of the theory

[39] As opposed to deriving the data from theory. According to Slater (2002) and Reinhardt (2006), an important step for the acceptance of spectroscopic methods by organic chemists was the development of simple rules of data interpretation that did not require deep knowledge of the instruments’ theoretical underpinnings.

> unaffected, and of the way in which modern research, instead of being content with evidence of one kind, as were the older organic chemists with that of chemical reaction, draws it material from every side and from every branch of chemistry and physics.[40]

My interpretation of Sidgwick's comments is that the structure theory was *a priori* compatible with different possibilities for the physical realization of the linkages, and the new methods helped to identify their actual properties. Following the advent of NMR spectroscopy in the 1950s, other properties, like conformational isomerism and new stereochemical relationships between groups in a compound, were also discovered. Sidgwick's comment about the eclectic character of the new kinds of evidence provides further support for my claim about the new approaches to solving chemical problems that emerged in this period.

In summary, the Instrumental Revolution helped to realize the following possibilities. First, that structure could be known independently of reactivity. This advance also permitted the discovery of structural properties, like conformational isomerism, that are inaccessible by means of reaction data. Second, which properties, among the possible ones that bonds could have (given the abstract role accorded them by classical structure theory), bonds actually have. The discovery of these properties amounted to a further development of the theory, since it now had physical content. Each of these realizations was a major step forward for structural chemistry. But this progress depended on a transformation of chemists' capacity to act.

5 Conclusion

In this concluding section, I compare my Agency View to three agency-based conceptions of scientific practice: David Gooding's "semantic ascent" of the observer, Hasok Chang's "systems of practice," and Hans-Jörg Rheinberger's notion of experimental systems. In *Experiment and the Making of Meaning* (1990), David Gooding asked "how do observers ascend from the concrete, practical context of individual experience of particulars to the realm of discourse about shared experience in which generalization, argument and criticism are possible?"[41] His answer was that the meaning of scientific terms

[40] Sidgwick (1936), pp. 533-534.
[41] Gooding (1990), p. xiii.

emerged from scientists developing a shared understanding of the pre-verbal practices involved in the production and experiencing of phenomena. According to Gooding, an understanding of the context of actions and objects in which phenomena are experienced is a necessary condition for the meaningfulness of discourse about phenomena. As noted by Baird (2004), however, the metaphor of ascent implies a hierarchy of ultimate values, in which theory stands at the summit. Baird goes on to point out that "maneuvers in the material realm are central to the progress of science and technology." The restructuring of the chemist's agency described in section 3 is a form of such maneuvering. Thus, one might say that whereas Gooding reconstructs a "vertical" relationship between action and theory, this essay has attempted to reconstruct the "zig-zagging" between them that occurs when the application of propositional knowledge in experiment requires extensive maneuvering at the level of agency, which in turn makes possible advances at the level of theory, which can then inform new experiments, and so on.

The next notion for comparison is Chang's system of practice. Chang (2011, 2012) articulates an activity-based view of scientific practice. According to Chang, an 'epistemic activity' is "a coherent set of mental or physical actions (or operations) that are intended to contribute to the production or improvement of knowledge in a particular way, in accordance with some discernible rules."[42] This activity-based view is intended to encompass both intellectual and manual aspects of scientific work. Epistemic activities are generally practiced in relation to others, forming what Chang (2012) calls a 'system of practice.' A set of epistemic activities forms such a system when they are performed with a view to achieving certain aims.[43] As I acknowledged in the introduction, my focus on epistemic roles is inspired by Chang's systems of practice. The latter, however, have a holistic character in that theories and systems of practice tend to be tightly associated because systems of practice come with their own standards of correctness. In this regard, a system of practice is similar to a Kuhnian paradigm, a similarity Chang acknowledges.[44] On the view I have developed in this essay, however, theory and practice are not so tightly associated because the epistemic roles played by the agents depend on facts, contingent

[42] Chang (2011), p. 209.
[43] Chang (2012), p. 216.
[44] Chang (2012), p. 218.

relative to theory, about the state of scientific knowledge, the level of technology, as well as social and material factors. As a result, the development of theory and that of techniques do not necessarily have the same temporal dynamics—each has its own time, mechanism and rhythm of development. It follows that change and progress at the level of techniques will not necessarily track change and progress at the level of theory.

The final notion for comparison is Rheinberger's "experimental system," which he introduces to account for the generation of what he calls "epistemic things." An experimental system is the basic unit of structure in which scientists, especially experimentalists, practice their trade, while epistemic things represent the object and product of such practice. If they come to be used as research instruments themselves, they become "technical objects." Rheinberger claims that "I am not looking for a logic behind experiment. Rather, I am grappling with what must be seen, irreducibly, as the 'experimental situation.' In this situation, "there are scientific objects and the technical conditions of their coming into existence, there is differential reproduction of experimental systems, there are conjunctions of such systems, and graphematic representations."[45]

In emphasizing the experimental nature of scientific practice, Rheinberger often minimizes or even excludes the theoretical dimension of scientific practice. Accordingly, the analysis of scientific practice in terms of experimental systems and cultures is meant to "free the experiment from its subsidiary role in rationalistic accounts of theory development and theory change."[46] In contrast, my Agency View does not attempt to "free" experimental activity from theoretical activity but rather to locate it with respect to such activity. More fundamentally, the notion of agency cuts across theoretical and experimental activity. Theorizing is a form of agency, and indeed it might be possible to tell a story, similar to the one told here, about the mechanization of theoretical work through the introduction of computers.

In conclusion, the Agency View is not an attempt to provide a comprehensive perspective for reconstructing scientific practice. Rather, it is an attempt to address the question: what is the contribution of changes in scientists' agency to scientific progress? Put somewhat differently, what difference does the constitution of the human-instrument

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[45] Rheinberger (1997), p. 21.
[46] Rheinberger (1997), p. 138.

relationship make to scientific progress? The point is not to reach a better understanding of experimental activity *per se*, but rather to better understand how the long-term dynamics of scientific change are affected by the distribution of actions between humans and instruments and between the humans themselves.

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