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# On “the application of science to science itself:” chemistry, instruments, and the scientific labor process<sup>☆</sup>

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## HIGHLIGHTS

- The mid-20th century Instrumental Revolution in chemistry is analyzed using a comparative approach.
- A Marxian analysis of mechanization processes in capitalist societies is employed.
- Organic chemical analysis before and after the Instrumental Revolution is compared.
- The role of machines in scientific change is emphasized.
- It is suggested that the episode may be an instance of a kind of revolution in science.

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## ABSTRACT

The “Instrumental Revolution” in chemistry refers to a transitional period in the mid-20th century during which sophisticated instrumentation based on physical principles was introduced to solve chemical problems. Historical and philosophical reflection on whether the revolution was a scientific one has been dominated by general models of scientific revolution, in particular, those proposed by Thomas Kuhn, I. B. Cohen and Ian Hacking. In this article I propose that the Industrial Revolution is a useful model for understanding the transformation wrought by the increasingly important role of machines in chemical research. Drawing on Marx’s analysis of that event, I argue that the Instrumental Revolution bears a striking resemblance to the industrial one. I offer grounds for thinking that the resemblance is not fortuitous, but rather reflects a general pattern of development involving the mechanization of the labor process. It is suggested that the cognitive consequences of radical changes in the means of production, as exemplified in the Instrumental Revolution, warrant the consideration of whether the latter is an instance of a kind of revolution in science rather than a singular episode.

## 1. Introduction

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 S. and Ann T. Tarbell,<sup>1</sup> 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 modern 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 molecular 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.

Historians writing about the Instrumental Revolution have advanced different views on whether and in what sense it might have been a genuine scientific revolution. On the side of those who think it was, Tarbell and Tarbell (1986) characterize it as the introduction of more powerful methods of purification and structure proof.<sup>2</sup> Morris and

<sup>☆</sup> The quotation is by the physicist Paul Klopsteg, whose advocacy for a science of “instrumentology”, in which scientific knowledge was to be applied systematically to the development of scientific techniques, will be mentioned below.

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<sup>1</sup> Tarbell and Tarbell (1986), ch. 21.

<sup>2</sup> Tarbell and Tarbell (1986), p. 335.

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Travis (2002), for their part, characterize it in Kuhnian terms, as the overthrow of the ruling paradigm by a new one.<sup>3</sup> Baird (2002), on the other hand, points out that the revolutionary phase of Kuhn's *Structure of Scientific Revolutions* starts with a crisis, when normal science encounters a problem that its established methods cannot solve.<sup>4</sup> Baird argues that at least as far as analytical chemistry was concerned, there was no such crisis. To the contrary, the new methods were developed in order to solve problems the established methods could already solve, but better—more efficiently, with smaller samples, greater sensitivity and lower limits of detection. Hence the Instrumental Revolution does not qualify as a revolution in Kuhn's sense.<sup>5</sup>

Baird goes on to examine other criteria for revolutionary status. First, he considers those advanced by I. B. Cohen (1985) in *Revolution in Science*. Baird finds that the episode does not fit Cohen's model for the stages of a revolution in science, which always begins with a private mental event. Such a model misses the core feature of the revolution, the introduction of an “instrumental-outlook” into the methods of analytical chemistry. Baird argues that a more promising model is to be found in Hacking's (1987) notion of a “big revolution”, which privileges wide-ranging changes in cultural practices and institutions in the search for scientific revolutions. Baird argues that the Instrumental Revolution fits Hacking's model, and therefore qualifies as a genuine scientific revolution.

On the side of the skeptics, Laszlo (2002) claims that there was no sudden change in the mid-20th century: the origin of organic spectroscopy should be located in the 1880s rather than the 1950s. Reinhardt (2006) concurs with Baird that the lack of anomalies and crises accompanying the changes disqualify it for the status of a Kuhnian revolution. He argues that the notion of an “Instrumental Revolution” neglects the “hidden continuities and step-by-step transition processes” that made the use of the new methods in chemistry possible.<sup>6</sup> According to Reinhardt, the key to assuring continuity was the emergence of a community of scientists, the “method makers”, who acted as mediators or “middlemen” for the importation of methods from physics to chemistry, by way of industrial instrument-makers. The upshot of Reinhardt's account is that the Instrumental Revolution failed to be a real revolution because the transfer of technology from physicists to ordinary chemists resulted neither in the reduction of chemical theory to physics nor in a loss of chemistry's disciplinary autonomy.<sup>7</sup>

The general models of scientific revolution that have dominated this discussion single out changes in theories, concepts, cultural practices and institutions, but are silent on how scientific practice is altered by the specific characteristics of machines, usually lumping scientific machines under generic categories like “instrument”.<sup>8</sup> But machines are not simply complex instruments. At least since the Industrial Revolution, they have tended to replace and displace human labor, which can have significant effects on the organization, and potential for technical progress, of the labor processes in which they are incorporated. The debate on the revolutionary status of the Instrumental Revolution has so far not considered the possibility that the revolutionary character of this event may lie in this specific characteristic of machines. Failure to do so may partially explain why neither Laszlo nor Reinhardt finds that the technology transfer brought about a revolution. Though the Tarbells note that “[t]he paucity of experimental methods and instrumentation available to organic chemists began to change with increasing speed in the 1930s”, they do not comment on the causes of the speed-up, other

than to point to discoveries in physics underlying the use of the new instruments.<sup>9</sup> Hacking's model posits four characteristics of “big revolutions” that have little to do with machines as such: discipline formation, the establishment of new social institutions like national science academies, large-scale social changes like the rise of capitalism, and changes in the “texture” of the world, such as when a probabilistic world-view displaced deterministic conceptions of the world.<sup>10</sup>

In this paper, I argue that the Instrumental Revolution bears a striking resemblance to the industrial one.<sup>11</sup> I begin by offering grounds for thinking that the resemblance is not fortuitous, but rather reflects a general pattern of development caused by the mechanization of the labor process, drawing largely on evidence from structural organic chemistry. Though my focus will be on the latter, I will also draw evidence from analytical chemistry, which in some ways was more profoundly affected because its professional identity was based on methods of analysis.<sup>12</sup>

My analytical approach here is inspired by two authors. First, I draw on philosopher Maurice Mandelbaum's notion of an ‘analogical approach’ to comparative historical studies.<sup>13</sup> This approach consists of two complementary subtypes. The ‘phenomenological form’ “rests on analogies drawn between instances that resemble one another with respect to certain overall characteristics of structure, such as the sequence of stages in revolutions, or some interrelated set of attributes that, taken together, are seen as constituting a specific ideal type.”<sup>14</sup> The phenomenological form can be complemented by the ‘analytical form’, which invokes underlying relationships in order to explain the similarities the phenomenological comparison merely describes. My ‘phenomenological’ claim in this paper is that the Instrumental Revolution resembles the industrial one with respect to eight structural properties that the two events have in common.

A few remarks on the intended scope of the analogy are in order here. I intend the analogy to apply to routine structure determination in organic chemistry. Since defining precisely what is meant by “routine” can be difficult, I will instead characterize it in terms of “subjective” and “objective” aspects. The subjective aspect of routine structure determination post-Instrumental Revolution is that it does not require, of the organic chemist, research and expertise on the methods, instrumentation, and theory of the instrumentation used to determine structures. I have in mind the kind of chemist who would be intended by the following statement of aims from a textbook on spectrometric identification of organic compounds:

We aim at a rather modest level of expertise in each area of spectrometry, recognizing that the organic chemist wants to get on with the task of identifying the compound without first mastering arcane areas of electronic engineering and quantum mechanics. But the alternative black-box approach is not acceptable either. We avoid these extremes with a pictorial, nonmathematical, vector-diagram approach to theory and instrumentation. Since NMR spectra can be interpreted in exquisite detail with some mastery of theory, we present theory in corresponding detail—but still descriptive.<sup>15</sup>

<sup>9</sup> Tarbell and Tarbell (1986), p. 335.

<sup>10</sup> Hacking (1987), pp. 50–52.

<sup>11</sup> For a discussion of the conceptual and semantic difficulties associated with the term “Industrial Revolution,” see Cohen (1985), ch. 17. In this paper, I use the term to refer to the transition from the period of manufacture to the period of large-scale industry in the 18th and 19th centuries, as analyzed by Marx in *Capital*.

<sup>12</sup> Baird (2002) argues that analytical chemists experienced a crisis of identity during this period.

<sup>13</sup> Mandelbaum (1984), pp. 135–139. I thank Professor James Lennox for making me aware of Mandelbaum's writings on the philosophy of history.

<sup>14</sup> Mandelbaum (1984), p. 138.

<sup>15</sup> Silverstein & Webster (1998), p. 1. I note in passing that the vector-diagram approach referred to in the quotation is a classical model of the bulk magnetization and therefore does not provide the accepted quantum mechanical

<sup>3</sup> Morris and Travis (2002), p. 80.

<sup>4</sup> Kuhn (1970).

<sup>5</sup> Baird (2002), pp. 47–48.

<sup>6</sup> Reinhardt (2006), p. 9.

<sup>7</sup> More recently, Gerontas (2014) has favored a Hacking-style interpretation and Chamizo (2018) an interpretation in terms of an extended Kuhnian model.

<sup>8</sup> For instance, Cohen (1985) calls both Galileo's telescope and the computer “instruments” in his discussion of their revolutionary effects on science. Cohen (1985), pp. 9–10.

The objective aspect is that the instruments have to be black-boxed, in the sense of Latour (1999) who defines black-boxing as:

An expression from the sociology of science that refers to the way scientific and technical work is made invisible by its own success. When a machine runs efficiently, when a matter of fact is settled, one need focus only on its inputs and outputs and not on its internal complexity.<sup>16</sup>

The invisibility of the machine's internal complexity makes it capable of being operated by someone who is not an instrument expert. Indeed, it is precisely this capability of the instruments discussed in this paper that makes possible the black-box approach resisted by the textbook quoted above. For example, another textbook claims that “[i]t is possible to treat the NMR spectrometer as a ‘magic box’ and simply memorize a few rules that suffice for deducing the structure of a compound from its spectrum.”<sup>17</sup> My focus on black-boxed instruments entails that I will be concerned with the use of standard tools like a tabletop infrared spectrometer rather than with that of a high-end research instrument like a 1 GHz NMR machine.<sup>18</sup>

These constraints on the scope of the analogy exclude, for example, researchers who use NMR to study large biological macromolecules, which does indeed require mastery of, and research on, the methods, instrumentation and theory of the instrumentation. I will also not be concerned with the methods used to produce the final instrument commodities (e.g., mass production versus custom manufacture) nor with extending the analogy to the social groups involved in the research, development and production of the instruments.

My second inspiration is Marx's analysis of the Industrial Revolution, which I draw on to formulate my ‘analytical’ claim. Unlike traditional Marxist historiography of science, however, my concern here is not primarily with the social origins of a particular scientific development.<sup>19</sup> Rather, I focus on changes in the labor process internal to the field. In *Capital*, Marx argues that the extensive, rapid and indefinite application of science and technology to productive processes under capitalism was made possible by the emancipation of factory production from the limitations imposed by native human abilities. This emancipation was brought about by the modification of the labor process, in particular the modification of what I will call “strategic functions” within the process. The modification of the function of tool-bearing in particular permitted a sequence of further transformations that exploited science and technology. My analytical claim is that something similar happened in chemistry, namely that the Instrumental Revolution also involved the emancipation of data production from the limitations imposed by humans' native epistemic abilities. The strategic function in this case was that of *detection*.

The paper is organized as follows. I describe structure determination before and after the Instrumental Revolution in section 2. In section 3, I describe Marx's analysis of the evolution of technology under capitalism. In section 4, I lay out my phenomenological claim, focusing on analogies and disanalogies between the Industrial and Instrumental Revolution. In section 5, I make the case for the analytical claim. In section 6, I address objections to my interpretation of this episode. I offer concluding remarks on the value of the analogy for the study of

(footnote continued)

explanation of NMR phenomena in terms of superposition states and product operators. It is nevertheless useful for teaching the kind of qualitative understanding the authors are aiming at.

<sup>16</sup> Latour (1999), p. 304.

<sup>17</sup> Streitwieser, Heathcock, and Kosower (1992), p. 325.

<sup>18</sup> I thank an anonymous reviewer for these examples. The reviewer further points out that the difference between these sorts of instruments is similar to that between the production and use of a Toyota Corolla and a formula racecar.

<sup>19</sup> For an overview of 20th century Marxist historiography of science, see Hadden (1994), ch.1.

scientific change, insofar as it affects the nature of scientific work, in section 7.

## 2. Structure determination before and after the instrumental revolution

In general, the goal of structure determination is to determine the connections between atoms in a molecule, and often the geometric properties of the molecule as well. With the acceptance of chemical structure theory in the late 19th century, chemists could turn the observations furnished by chemical reactions into evidence for molecular structure.<sup>20</sup> 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 awarding of Nobel prizes.<sup>21</sup> A famous example is strychnine, which was isolated in 1815 but whose structure was not definitively established until 1948 despite intensive efforts to do so: at least 245 papers were contributed to solving it from the time of strychnine's isolation to 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.”<sup>22</sup>

Classical chemistry was heavily dependent on the performance of manual work by the chemist.<sup>23</sup> 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 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.<sup>24</sup>

In contrast with these 19th-century methods, the Instrumental Revolution ushered in new techniques based on physics, notably

<sup>20</sup> 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.

<sup>21</sup> A list is provided in Morris and Travis (2002), p. 60.

<sup>22</sup> “The Nobel Prize in Chemistry 1947”. Nobelprize.org. Nobel Media AB 2014. Web. [http://www.nobelprize.org/nobel\\_prizes/chemistry/laureates/1947/](http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1947/). (Accessed 24 July 2015). See Slater (2001) for an account of the strychnine research.

<sup>23</sup> 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.

<sup>24</sup> Knight (2002), pp. 87–90; cf. Tarbell and Tarbell (1986), p. 335. Knight's comment about apparatus agrees with Jackson's (2015a,b) 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).

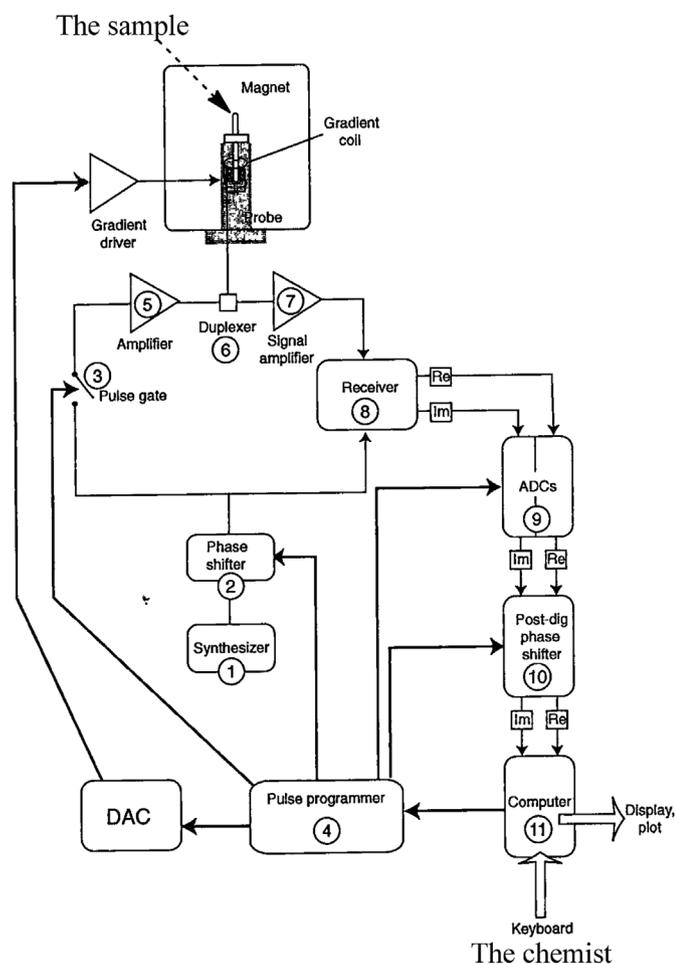


Fig. 1. The scene of the “crime”: a schematic overview of a pulsed-field NMR spectrometer. Source: Levitt (2008, p. 81).

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  $^1\text{H}$  and  $^{13}\text{C}$  nuclei. A schematic of an NMR spectrometer is shown in Fig. 1. 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.

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 methods were based on science and technology with which chemists were largely unfamiliar. The instruments required were also very expensive. Nevertheless, there was a significant pay-off for adopting the methods. Structure determination became much more efficient, freeing up the chemists’ time for other work, such as synthesis

(which was not mechanized and where chemical expertise remained absolutely essential) 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,<sup>25</sup> only 6 were required over 5 years for the independent solution of the X-ray structure (Fig. 3).<sup>26</sup>

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 it. The means he employed were chemical reagents, glassware and auxiliary tools like balances, 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. The success of chemical research was heavily dependent on manipulative skills, as noted by Faraday in 1827.<sup>27</sup> 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 substance’s reactivity.<sup>28</sup> 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.<sup>29</sup>

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.”<sup>30</sup> 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.”<sup>31</sup> In modern chemistry, structures are determined by inserting an isolated sample into such systems. The chemist is generally not the designer of the instrument. In routine use, she or he must prepare the sample, choose the kinds of experiment to use, operate the instrument, and interpret the spectrum, though in routine cases these operations are fairly standard.<sup>32</sup> Her chemical laboratory skills are limited to sample preparation, for example dissolving the sample in an

<sup>25</sup> Huisgen (1950).

<sup>26</sup> See the primary sources cited in Slater (2001), footnote 78.

<sup>27</sup> Faraday (1974), iii.

<sup>28</sup> For an example of how evidence for a structural hypothesis was developed in classical chemistry, see Slater’s (2001). Sir Robert Robinson has many examples in his (1976) autobiography. The textbooks by Mulliken (1904) and Shriner, Fuson, and Curtin (1956, 3rd ed.) provide a systematic overview of classical methods.

<sup>29</sup> 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 and Allinger (1965), p. 36.

<sup>30</sup> Rothbart and Slayden (1994), p. 29.

<sup>31</sup> Rothbart and Slayden (1994), p. 37.

<sup>32</sup> For certain techniques, such as X-ray crystallography or high-resolution mass spectrometry, these operations are often carried out by instrument specialists rather than by the chemists who isolate the substance to be analyzed.

(a)



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Fig. 2. Instrument advertisements are interesting for what they reveal about how the makers conceived the relationship of the user to the machine. (a) A 1968 Varian Associates advertisement stressing ease of operation announces an NMR spectrometer for routine use by the average chemist. Source: *Analytical Chemistry*, 40, 125A. (b) With the help of a sexist double-entendre, Varian emphasizes that the chief locus of "activity" is in the machine rather than the human operator. Source: *Analytical Chemistry*, 1979, 50, 933A. It should be noted that, contrary to what the juxtaposition with Fig. 1 might suggest, the Varian T-60 had neither a superconducting magnet nor a pulse programmer. On the other hand, the XL-200, introduced in 1978, was equipped with both components.

appropriate solvent or crystallizing the substance.

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. Though chemical skills are involved in sample preparation, the production of information from the sample depends not

on them but on whether this orchestration of systems is such as to produce a reliable signal.

Thus the new instruments did not transfer the skills needed for classical structure determination to the machine. Rather, they substituted a new process for the old one. In the new process, the goal of structure determination was attained without the use of chemical reactions. This is an instance of what Keating, Limoges and Cambrosio (1997) call 'automation.' According to them,



significantly from the usual notion, as the use of a machine to substitute for human action by mimicking the latter through mechanical operations. For Keating, Limoges and Cambrosio, the automated process may involve operations that are quite different from—do not mimic—the human one. In addition, they do not simply replace humans but rather change the kinds of actions performed by humans. Automation through mimicry is merely a special case of this more general kind of automation. Nevertheless, I think the usual notion of automation as mechanical mimicry is still useful because it indicates an essential feature of automation, which is that some phases of the production process are delegated from humans to machines. Moreover, these phases must happen “automatically,” i.e. the machine must be able to carry out tasks without human intervention. But the manner in which the machines carry out those phases can be quite different. In the chemical case, the thing produced was a structural representation of a compound (as in Fig. 1a), 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. Marx's analysis of the labor process and the industrial revolution

As suggested by my reference to the “labor process”, my view starts from the assumption that science can be accurately conceptualized as a material labor process, similar in important respects to ordinary labor processes.<sup>34</sup> In this article, I draw on Marx's analysis of the mechanization of industrial labor processes during the Industrial Revolution because the pattern of development of the Instrumental Revolution in certain respects fits rather well the pattern described in his analysis. I will restrict myself here to summarizing the key methodological points required for understanding my position. It should also be noted that what I take from Marx is conceptual rather than empirical. Hence I will be concerned with his way of conceptualizing what made the technical changes during the Industrial Revolution possible, and not with the truth of his empirical claims concerning the course of technical change in capitalist economies during the 18th and 19th centuries, except insofar as these affect the cogency of the conceptualization.<sup>35</sup>

The non-Marxist 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.”<sup>36</sup> One question this claim raises is what makes the extended application of science to production possible? An obvious answer is the growth of scientific knowledge. But as economist Nathan Rosenberg noted in his interesting (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.<sup>37</sup> To believe that is to ignore the mediating role of technology in the production process. Marx himself characterizes the labor process in general in terms of three simple elements:

The simple elements of the labour process are (1) purposeful activity (*zweckmässige Tätigkeit*), that is work itself, (2) the object on which that work is performed, and (3) the instruments of that work.<sup>38</sup>

Technology, in the form of the instruments of labor, mediates the process of transforming the object of labor and hence of realizing the

worker'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?<sup>39</sup>

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 dynamism 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,<sup>40</sup> 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.<sup>41</sup> This “principle” encountered the limitation that:

Whether complex or simple, each operation has to be done by hand, retains the character of a handicraft, and is therefore dependent on the strength, skill, quickness and sureness with which the individual worker manipulates his tools. Handicraft remains the basis, a technically narrow basis which excludes a really scientific division of the production process into its component parts, since every partial process undergone by the product must be capable of being done by hand, and of forming a separate handicraft.<sup>42</sup>

Rosenberg sums up the problem neatly:

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.<sup>43</sup>

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.”<sup>44</sup> The worker's skills can now be replaced by non-human 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.”<sup>45</sup> 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.<sup>46</sup>

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 abilities?<sup>47</sup> But

<sup>39</sup> Rosenberg (1981), p. 15.

<sup>40</sup> Marx (1976), p. 455.

<sup>41</sup> Marx (1976), p. 501.

<sup>42</sup> Marx (1976), p. 457.

<sup>43</sup> Rosenberg (1981), p. 16.

<sup>44</sup> Rosenberg (1981), p. 16.

<sup>45</sup> Marx (1976), pp. 590, 616–617.

<sup>46</sup> Marx (1976), pp. 505, 508–509.

<sup>47</sup> The term ‘native human ability’ is somewhat of a misnomer, since very few of our abilities are completely native, in the sense of resulting solely from our biological endowment. Most human abilities require socialization and education, as well as material means. I discuss this notion in more detail in Borg (forthcoming).

<sup>34</sup> For a recent defense of this assumption, see Lefèvre (2005).

<sup>35</sup> That said, those aspects of Marx's account of the Industrial Revolution that I will use here appear to be in broad agreement with more recent scholarship. See Allen (2017), especially ch. 3 on “Why the Industrial Revolution was British” and the references cited therein.

<sup>36</sup> Kuznets (1966), p. 9.

<sup>37</sup> Rosenberg (1981), p. 15.

<sup>38</sup> Marx (1976 [1867]), p. 284; (1959), p. 193 for the original German.

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 “mechanisms”:

The machine, which is the starting-point of the industrial revolution, replaces the worker, who handles a single tool, by a mechanism operating with a number of similar tools and set in motion by a single motive power, whatever the form of that power.<sup>48</sup>

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.

My suggestion, based on this analysis, 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 to about 1300 CE, 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 of 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 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.<sup>49</sup>

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 separable 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.

There can be more than one strategic function in a given production process. Rather than modify the tool-bearing function, for example, employers in the manufacturing period preferred to modify the operations performed by the worker. According to Marx's account, this modification began with the decomposition of a single process formerly performed by a single craftsman into simpler operations, each performed by a specialized worker. Though the initial effect is simplification, specialization eventually leads to perfecting the methods and skills of the worker. Specialization also increases productivity by eliminating transitions from one partial operation to another. The full exploitation of the specialization of labor requires changes in the instruments of labor, for these must be adapted to the new skills. Furthermore, splitting up the original process into partial operations allows the latter to be carried on simultaneously, leading to a further

gain of total productivity. Since the partial operations are performed by different workers, the continuity of the overall process depends on each worker spending no more time than necessary to complete his or her designated function, leading to an increase in efficiency. Finally, specialization allows differences among individuals to be developed, insofar as some will specialize in operations requiring more strength, others more skill, attention, intellectual effort, etc. All of these changes in the nature of the work, however, were made possible by the initial simplifying decomposition.<sup>50</sup>

Clearly, any significant process of technical change will involve more than is suggested by these sorts of linear descriptions. Moreover, not all changes in work may be amenable to an analysis in terms of strategic functions at all. I merely suggest that, in some cases, it may be a useful analytical concept.

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 section 5, I will argue that detection played the role of a strategic function in chemical analytical instrumentation.

Finally, it should be noted that 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 the “principle of machine production”, cognitively involved the discarding of this assumption:

In manufacture, it is the workers who, either singly or in groups, must carry on each particular process with their manual implements. The worker has been appropriated by the process; but the process had previously to be adapted to the worker. This subjective principle of the division of labour no longer exists in production by machinery. Here the total process is examined objectively, viewed in and for itself, and analysed into its constitutive phases. The problem of how to execute each particular process, and to bind the different partial processes together into a whole, is solved by the aid of machines, chemistry, etc. But of course, in this case too, the theoretical conception must be perfected by accumulated experience on a large scale.<sup>51</sup>

The principle of machine production, namely the division of the production process into its constituent phases, and the solution of the problems arising from this by the application of mechanics, chemistry and the whole range of the natural sciences, now plays the determining role everywhere.<sup>52</sup>

It is worth noting that the “principle of machine production” does not refer narrowly to production by means of devices that mimic human action (e.g., by bearing tools), but involves a problem-solving approach that draws on the entire store of scientific and technological knowledge. This approach was not employed by the direct operators on the factory floor (often relatively unskilled workers, including women and children) but rather by the owners and designers of the instruments: capitalists, inventors, engineers, etc. 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. I will 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.

<sup>48</sup> Marx (1976), pp. 497.

<sup>49</sup> Hills (1990), pp. 808–830; Usher (1954), ch. XI, section VI; Fitton and Wadsworth (1958), pp. 211 (photograph facing) and p. 217.

<sup>50</sup> Marx (1976), ch. 14.

<sup>51</sup> Marx (1976), p. 501.

<sup>52</sup> Marx (1976), p. 590.

In short, what I take from Marx's 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 and technological 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.

#### 4. Parallels between the industrial revolution and the instrumental revolution

In this section, I discuss two sets of evidence suggesting a relationship between the Instrumental Revolution and the Industrial one. First, the conceptions of progress of some of the participants in the Instrumental Revolution were formulated in terms of features characteristic of industrial production. Second, the two events share eight common features with respect to how their respective labor processes were altered.

##### 4.1. Conceptions of progress

In some cases, the Instrumental Revolution was actually characterized by the participants in terms alluding to large-scale industry and the use of machines outside of science. For example, John K. Taylor of the Center for Analytical Chemistry at the National Bureau of Standards commented in 1985:

Chemical analysis is undergoing a change of operational mode similar to the industrial revolution of a century ago ... The trend is from individual craftsmanship to mechanical outputs, using apparatus and equipment that is often poorly understood by the technical operator.<sup>53</sup>

In the forward to a book on the DENDRAL project, an attempt to automate structure elucidation by mass spectrometry, the noted organic chemist Carl Djerassi wrote in 1980 that “[i]t is [in synthesis] where the use of computers has not been widely accepted because of the fear that thinking man will simply be reduced to an appendage to a machine.”<sup>54</sup> Joshua Lederberg, one of the project leaders, dreamt of “mechanizing” scientific thinking in biology and organic chemistry and reducing the human role to one of management:

If we could give biology sufficient formal structure, it might be possible to mechanize some of the processes of scientific thinking itself ... Could not the computer be of great assistance in the elaboration of novel and valid theories? We can dream of machines that would not only execute experiments in physical and chemical biology but also help design them, subject to the managerial control and ultimate wisdom of their human programmer.<sup>55</sup>

Comparisons to instruments used outside of science were also made. For example, Djerassi compared X-ray diffraction to the flash camera, and the analytical chemist H. A. Liebhafsky drew an analogy between the introduction of the new instruments and the mechanization of artillery, judging such “revolutions” to be “necessary.”<sup>56</sup>

Such quotations provide grounds for thinking that participants in the Instrumental Revolution were influenced by ideas derived from examples of mechanization in the broader society. In the next

subsection, I will show that their ideas corresponded to structural similarities between the two events.

##### 4.2. Common features

I have identified eight features common to both events, considered as transformations of their respective labor processes:

###### 4.2.1. *The labor process no longer uses means and methods borrowed from an antecedently existing activity. It acquires means and methods specifically adapted to its purpose*

Classical structure determination found its means ready-made in the technology of substance manipulation. These means had several drawbacks for the productivity of structure determination, including drawbacks such as that: large amounts of substance were required; the processes employed were time-consuming; the variety of evidence for structural claims was poor; and the principal evidence used, that provided by chemical properties, tended to underdetermine the structures identified by means of it. Consequently, the development of the productivity of structure determination required that means better suited to this end be found. Spectroscopic methods were very effective for this purpose: they require only small amounts of substance; they are rapid; they come in many varieties; and they are better at uniquely identifying functional groups and connectivities. Analogously, during the Industrial Revolution, capitalists transformed the production processes they had inherited from the medieval handicrafts to fit the needs of a capitalist economy, in particular the need to increase profits without increasing the length of the working day. This was achieved by increasing productivity through technological innovation.<sup>57</sup>

###### 4.2.2. *The labor process becomes centered around an instrument rather than the worker*

As I discussed in section 2, classical structure determination was essentially based on the chemical laboratory skills of the chemist. These skills are marginalized in modern structure determination. The labor process is now essentially based on machines. While methods developers focus on optimizing the functioning and extending the scope of the machines, the average user types in standardized instructions at the computer.<sup>58</sup> Experimental design, optimization and execution become based around the ability of a specific kind of machine to carry out a process that associates a specific kind of input with a specific kind of output.

###### 4.2.3. *The work becomes more capital-intensive*

A report published by the National Academy of Sciences in 1965 estimated the typical cost of a high resolution NMR spectrometer at \$45,000, or \$355,563 in 2017 dollars.<sup>59</sup> The total approximate investment in instrumentation by all university chemistry departments rose from \$5 million before 1954, to \$14 million in the period 1954–1959, to \$36 million for the period 1960–64 alone, resulting in a total accumulated investment of \$55 million. In comparison, the report estimates that a total of \$31 million was spent on traditional equipment (glassware, vacuum pumps, variacs, supplies, chemicals etc.) during the same periods.<sup>60</sup> Thus there is evidence that even when the new instrumentation was still novel, expenditures on it outstripped traditional kinds of expenditures by a wide margin. The problem of rapid

<sup>57</sup> Marx (1976), ch. 12.

<sup>58</sup> Reinhardt (2006) emphasizes the emergence of the methods developers as a distinct scientific community.

<sup>59</sup> National Academy of Sciences (1965), p. 216. 2017 price calculated using the U.S. Bureau of Labor Statistics inflation calculator, based on the Consumer Price Index.

<sup>60</sup> National Academy of Sciences (1965), pp. 97 and 216. Reinhardt (2006), pp. 382–386, contains a brief discussion of investment trends in research chemistry from the 1950's through the 1970s.

<sup>53</sup> Taylor (1985), p. 6.

<sup>54</sup> Djerassi (1980), ix.

<sup>55</sup> Lederberg (1969), p. 38.

<sup>56</sup> Djerassi (1992), p. 84; Liebhafsky (1962), p. 32A.

obsolescence of equipment and the attendant funding burden emerged in chemistry at this time.<sup>61</sup>

#### 4.2.4. *The worker is not a specialist of the instrument*

One of the principal themes of Reinhardt's (2006) study of the Instrumental Revolution is that specialists developed methods enabling non-specialists to use the instruments.<sup>62</sup> This development resembles the use of workers in large-scale industry who had little knowledge of the scientific principles embodied in their machines. Methods developers had to create cognitive methods, like the rules of interpretation mentioned in the following subsection, so chemists, as routine users, could interpret the data without detailed knowledge of the science on which their instrumentation was based. In addition, textbook writers incorporated simplified theoretical treatments, connecting the workings of the machines with chemical concepts, into chemistry textbooks.<sup>63</sup>

#### 4.2.5. *Specialized labor is replaced by non-specialized labor*

Before the Industrial Revolution, capitalist production was based on the specialized labor of the handicraftsman; afterwards, it was based on the non-specialized labor of the machine-operator. Similarly, before the Instrumental Revolution, structure determination was based on the chemical skills of the chemist, whereas afterwards it was based on her ability to operate the machines using procedures and rules of interpretation adapted for non-specialist use.<sup>64</sup> The training times required to learn how to operate the machines are disproportionately short, compared either to the amount of knowledge embodied in them, or to the amount of time required to train a competent bench chemist (several years). For example, the website of the NMR facility of the University of Pittsburgh states that “a little more than an hour” is required to train a user in running basic 1-dimensional NMR experiments, 45 min for familiarization with basic 2-dimensional experiments, and 20 min for variable-temperature training.<sup>65</sup> And the Varian advertisement in Fig. 2a promises a 15 min training time ...<sup>66</sup>

The interpretation of the signal itself often involves no more than the use of rules that can be applied to read off structural features from

the spectrum. Fig. 4, for example, shows the result of one of the first attempts to correlate spectroscopic properties (here, infrared absorption) with structure. Having obtained the IR spectrum of a substance, the chemist can correlate each peak in the spectrum with functional group constituents by scanning along the abscissa, locating the wavenumber of the peak, and then scanning along the ordinate to identify the functional groups that are correlated with that wavenumber. The interpretation of spectra in this fashion is an instance of what the physical chemist J. P. C. Schwarz called an ‘empirical approach’ to the use of the new instrumentation. This approach depended on “the empirical correlation of certain physical properties with structural features.” He contrasted this way of interpreting spectra with a ‘theoretical approach’, in which structure is deduced by interpreting the data in terms of the theories justifying the use of the instruments.<sup>67</sup>

#### 4.2.6. *Automation becomes a significant feature of the production process (of goods, data)*

Though the chemist must still prepare the sample, beyond this, routine use of the machines requires only insertion of the sample and the feeding of standard instructions to the instrument. In 1999, Djerassi commented on the introduction of X-ray crystallography into structure elucidation work in blunt terms: “If anyone can prove a structure with an X-ray analysis, we are nothing. The organic chemist is nothing but a little technician who crystallizes the compound and gives it to someone who sticks it in an X-ray machine, and even the rest is computerized. So what's your function?”<sup>70</sup> Though Djerassi no doubt exaggerates the degree of automation brought about by the new methods, especially with respect to X-ray crystallography, the context of the quotation is comparative: as discussed in section 2, human manual intervention in the production of the data is greatly reduced relative to classical chemical manipulations. Both this feature and 4.2.4 above are succinctly expressed in the following NMR textbook:

It is one of the great virtues of NMR spectroscopy that one can use it, and indeed use it to quite a high level, without having the least idea of how the technique works. For example, we can be taught how to interpret two-dimensional spectra ... in a few minutes, and similarly it does not take long to get to grips with the interpretation of NOE ... difference spectra. In addition, modern spectrometers can now run quite sophisticated NMR experiments with the minimum of intervention, further obviating the need for any particular understanding on the part of the operator.<sup>71</sup>

#### 4.2.7. *The cognitive and physical limitations of humans are circumvented by advances in instrumentation design*

Methods developers could now attempt to circumvent the limited cognitive and physical abilities of humans by developing the machines' computational power, automation and versatility as well as the quality and variety of the data. For example, James Shoolery of Varian Associates commented in 1995 that the introduction of programmable computers into NMR spectrometers in the late 1960s allowed a control of the instrument with:

a speed and precision far beyond the capability of a human operator. Freed from those limitations, the development of NMR as a structural and analytical tool soon entered an exciting new period.<sup>72</sup>

The options for circumventing human limitations were significantly

<sup>61</sup> Liebhafsky (1962), 27A.

<sup>62</sup> Cf. also Gerontas (2014).

<sup>63</sup> Slater (2002) discusses R. B. Woodward's pioneering role in the development of rules of interpretation in the context of ultraviolet spectroscopy. See also Morris and Travis (2002) and Reinhardt (2006) for discussions of the textbooks produced during this period. The simplified theory together with the instruments resemble what Fujimura (1988) calls a “standardized package” of theory and technology whose widespread adoption results in a “scientific bandwagon.”

<sup>64</sup> On the process of adaptation, see in particular Rabkin (1988,1993), Bigg (2002) and Reinhardt (2006).

<sup>65</sup> <http://www.chem.pitt.edu/facilities/nmr-spectroscopy/training>. (Accessed July 22, 2015).

<sup>66</sup> Though advertisements are not impartial sources, that the principle techniques discussed in this paper had either been routinized or were in the course of routinization by the early 1960s (the Varian advertisement is from 1968) is supported by textbooks of the period [Schwarz (1964), pp. 2–3; Silverstein and Bassler (1963), p. 2]. It is also supported by the manner in which the instruments were developed. In NMR, for example, a major impediment to non-specialist use was the instability of the magnetic fields that could be generated in the 1950s, which required individual calibration and duplication of each spectrum. This problem was overcome by the introduction of the field/frequency lock technique. The first commercial use of this technique was in the Varian A-60 spectrometer, which included a number of other design features that were intended to facilitate routine use by structure elucidation chemists. According to Becker, Fisk, and Khetrapal (1995), pp. 35–37, the instrument was a success, bringing NMR “to almost every chemistry laboratory as a standard analytical method.” The role of the A-60 in routinizing and disseminating NMR is corroborated by Lenoir and Lécuyer (1995) and Steinhauser (2014), pp. 127–132 and p. 381. I thank two anonymous referees for pressing the point concerning advertising.

<sup>67</sup> Schwarz (1964), pp. 3–4.

<sup>68</sup> Slater (2002), Reinhardt (2006).

<sup>69</sup> Colthup (1950), pp. 398–399.

<sup>70</sup> Quoted in Reinhardt (2006), p. 170.

<sup>71</sup> Keeler (2010), p. 1. See also Streitwieser et al. (1992), p. 325.

<sup>72</sup> Shoolery (1995), p. 44. Grayson (2004) provides evidence that the computer came to play a similarly central role in mass spectrometry.

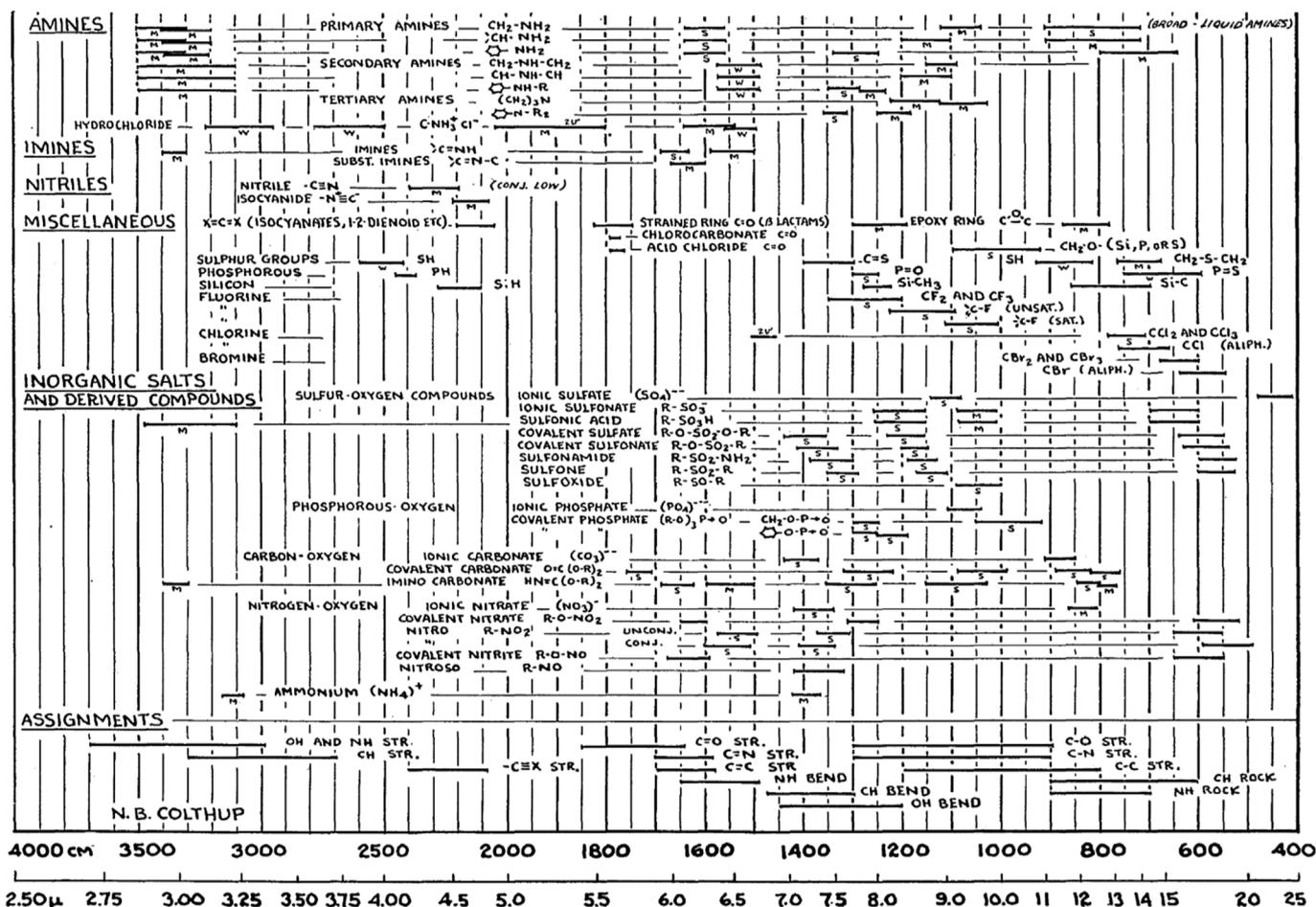


CHART 1. Probable positions of characteristic infra-red absorption bands.

Fig. 4. An important step for the acceptance of spectroscopic methods by organic chemists was the development of simple rules of data interpretation.<sup>68</sup> These rules were often presented in the form of charts allowing the chemist to correlate, at a glance, the observed frequencies with the presence of functional groups in the molecule. Shown above is a portion of the first such chart, published by Norman Colthup of American Cyanamid in 1950.<sup>69</sup>

fewer in classical chemistry, resulting in a relatively conservative pattern of methodological development. This conservatism was illustrated in section 2 by the testimony of David Knight.<sup>73</sup> Likewise, once the tool-bearing function was transferred from man to machine, industry could use more powerful motive powers than humans to drive the machine and its tools.<sup>74</sup>

#### 4.2.8. The transformation is motivated in part in terms of productivity norms—the speed, ease, simplicity, reliability and automaticity of the new techniques

An interesting aspect of the Instrumental Revolution is that industry pioneered the use of modern spectroscopic instrumentation in order to boost productivity before the instrumentation became widespread in academic chemistry.<sup>75</sup> Efficiency considerations were also adduced by academic proponents of the new methods. The physicist Paul Klopsteg, to whom the analytical chemist Ralph Müller referred in his influential 1940s column on instrumentation,<sup>76</sup> made efficiency the principal

theme of his 1945 *Science* article on “Increasing the Productivity of Research”. Commenting on the rapid recent development of instrumental methods across the sciences, Klopsteg argued for the establishment of laboratories of “instrumentology” in universities in order to increase “the output of valuable results per dollar.” Instrumentology was to be a science whose goal was “the application of science to science itself.”<sup>77</sup> The chemists Silverstein and Bassler, authors of the widely used textbook *Spectrometric Identification of Organic Compounds*, argued in 1962 that the cost of the instrumentation was outweighed by the speed, small sample size and large informational pay-off made possible by it, as well as by its increasing simplicity.<sup>78</sup>

Such productivist goals were also supported by university administrations. In the context of the Cold War, ambitious administrators could aim to maximize the output of research and graduate students by drawing on the large amounts of state and industrial funding that were then available. For example, Carl Djerassi did his pioneering work in

<sup>73</sup> Tarbell and Tarbell (1986), p. 335 and Taylor (1985) make similar observations.

<sup>74</sup> Marx (1976), pp. 497–499.

<sup>75</sup> See Rabkin (1988), Bigg (2002) and Reinhardt (2006) for accounts of the “detours” taken by ideas originating in physics through industry before reaching chemistry.

<sup>76</sup> Müller (1947), p. 24A. See Baird (2002) for a discussion of Müller’s role in the Instrumental Revolution in analytical chemistry in the 1940s.

<sup>77</sup> Klopsteg (1945), p. 571–572. Italicized in the original.

<sup>78</sup> Silverstein and Bassler (1962), p. 547. See also Reinhardt (2006) for comments by John D. Roberts and William S. Johnson (both important proponents of the instrumental approach) as well as Djerassi on the labor-saving virtues of the new methods (Reinhardt, 2006, pp. 20 and 157). The scientific testimony and textbook comments in the references in footnote 28 above all compare the difficulty of classical structure determination to the relative ease, simplicity or rapidity of the modern. See also the comment by S. Z. Lewin in section 4.3.

mass spectrometry at Stanford, after moving there from Wayne State University at the invitation of ambitious provost of Stanford Frederick E. Terman. Terman was committed to developing the university in directions that would attract funding agencies and industrial companies, and had a new building built to house both Djerassi's group as well as that of Djerassi co-hire William S. Johnson. Djerassi set up a research group organized around an assembly of physical instrumentation and structured by a strict division of labor. Wet chemists supplied compounds, technicians ran the instruments, “computers”—wives of graduate students at first, then artificial computers—processed the data, and senior post-doctoral fellows interpreted the spectra.<sup>79</sup> In his memoirs, Djerassi characterized the vision he had for his lab during the move as that of a “quasi-socialist enterprise” run by a “benevolent dictator”, possibly reflecting the influence of external methods of organizing labor on his thinking.<sup>80</sup>

Those who resisted the mechanization of structural chemistry found ammunition in efficiency as well. For example, Sir Robert Robinson thought the time saved by the new methods was illusory, for they revealed no chemical properties.<sup>81</sup> Likewise, some chemists who focused on the pedagogical consequences of the instrumental methods were concerned that the education of chemists would suffer if too much of the curriculum was devoted to the new methods, for the latter saved time at the expense of properly chemical training.<sup>82</sup> Such pedagogical reflections are especially interesting in light of what was said in section 3, for they underscore the fact that some classical chemists did not view structure determination merely as a process for accumulating known structures, but also as a process of apprenticeship.

#### 4.3. Disanalogies

As with any analogy, there are respects in which this one breaks down. The transformation of labor affected only one, albeit important, activity, though there are efforts currently afoot to mechanize synthesis as well.<sup>83</sup> Chemistry never became Big Science, but largely continued to favor small-scale projects. The delegation of expertise to specialists was not total, since some knowledge of how the instruments work remained desirable for data interpretation. And as noted in section 2, there was no attempt to mechanize the tools of classical chemistry.

Perhaps the most important disanalogy has to do with the social groups driving the change. As pointed out 4.2.1 above, during the Industrial Revolution capitalists transformed production processes to increase profits through technological innovation. It is unclear who the equivalent actors to the capitalists might be in the chemical case, or what goal plays the role of profit. With respect to the actors, previous studies on the introduction of the instrumental methods in chemistry show that the actors were small instrument manufacturers, research technologists,<sup>84</sup> scientists working as method makers or lead users, officers of funding agencies, and university administrators. This motley group of actors is very different from the owners of the means of production central to Marxist theory. Though profit certainly motivated the manufacturers, it is doubtful that it was as important a motivation to the other members of the group. Prestige would seem to be more important in these cases.

It might also seem like a stretch to compare 20th century organic chemists to early industrial factory workers. I only claim, however, that in both cases, mechanization allowed the operators to treat the new

instruments more or less like black-boxes. The import of the analogy with the Industrial Revolution is that the latter represents a repeating pattern in the development of technology in Western capitalist societies. Moreover, a possible, and sometimes actual, long-term effect of automation in industry is to “free up” workers for labor-intensive kinds of production. This is analogous to what happened in chemistry, in the sense stated above, that chemists could now spend more time on other kinds of production like synthesis and applications. Of course, there is the disanalogy that in the industrial case, different groups of workers are employed in the labor-intensive versus the capital-intensive industries, whereas in the chemical case it is more complicated: in some research institutions the chemists operate the machines themselves for routine jobs, whereas in others, technicians take care of data production; in most cases there are instrument experts who maintain, improve and in some cases operate the instruments.

Moreover, increasing productivity was not the only reason for adopting the new methods. Scientific norms of accuracy and epistemic security were major motivations. That said, scientific justifications for adopting the new methods often seem to have been mixed in with, and even in tension with, productivity-related justifications. A 1958 review of the new instrumentation by physical chemist S. Z. Lewin of NYU is at pains to point out the scientific benefit over and above the increased productivity: “the process of collecting analytical data has been made quicker, pleasanter, and more effortless [by the new instruments]. That is, however, only a part—and a minor part, at that—of the new capacities these instruments have provided to the analyst.” It is worth noting that his target audience was analytical chemists.<sup>85</sup>

Furthermore, and as noted in the introduction, I have only been concerned with standard instruments and routine users. Scientists working at the cutting-edge of chemical analysis, say in protein structure determination, have very specific needs that require specialized instruments and the scientists to be experts in their instrumentation.

Despite these disanalogies, I think the eight common structural properties described above are suggestive of common underlying factors responsible for the common properties, and in the next section I will proceed to sketch hypotheses as to what these factors could be.

## 5. Explication of the analytical claim

Why might there be common structural properties between the mechanization processes described by Marx and the Instrumental Revolution? After all, the contexts are very different—one instance of mechanization occurring in the production of commodities, with examples drawn from the 18th and 19th centuries, the other in the production of data for chemists in the middle of the 20th century. It may seem implausible that the two instances have anything to do with each other.

Nevertheless, there is evidence that 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.”<sup>86</sup> The potential for applying NMR to structural problems other than relatively small molecules was not

<sup>79</sup> Reinhardt (2006), pp. 144–173.

<sup>80</sup> Djerassi (1992), p. 100.

<sup>81</sup> Robinson (1974), p. 57.

<sup>82</sup> E.g., Lingane (1948), p. 2; Shriner et al. (1956), pp. v–vi; and Silverstein and Bassler (1962), p. 546.

<sup>83</sup> E.g., Webb (2015).

<sup>84</sup> On the role of research technologists in 20th century chemistry, see Shinn (2002).

<sup>85</sup> Lewin (1958), p. 19A; see also 20A. The article is billed as a “report for analytical chemists.” See also Tishler (1983), p. 13 and footnote 59 above.

<sup>86</sup> Feeney (1999), pp. 206–207.

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.”<sup>87</sup> Scientific texts also display the principle at work.<sup>88</sup> In his call for the establishment of instrumentology laboratories, 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. Lewin's review also emphasizes the instrumentation's 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, and all those aspects of physics and chemistry that treat the interactions of radiant energy and electric or magnetic fields with matter.<sup>89</sup>

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 origin of the new instrumentation. 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.”<sup>90</sup>

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 to 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.<sup>91</sup>

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.”<sup>92</sup> 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.<sup>93</sup>

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.<sup>94</sup>

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.<sup>95</sup>

For some corroboration of Lewin's claims, I will briefly discuss the strategic role of detection in mass spectrometry.<sup>96</sup> 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, 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. This modification enabled automatic strip chart recording of the mass spectrum, which simplified and accelerated spectrum recording compared to the photographic method. Strip chart recorders yielded an analog recording, however, which had to be

<sup>91</sup> Lewin (1958), p. 19A.

<sup>92</sup> Lewin (1958), p. 19A.

<sup>93</sup> Lewin (1958), p. 22A (digitization is my example).

<sup>94</sup> Lewin (1958), p. 20A.

<sup>95</sup> 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 and Eklund (1997), p. 559, and Thackray and Myers (2000), pp. 149–151. For a skeptical view of the photocell's potential in the 1930s, see Twyman (1931). Twyman was the technical director of Adam Hilger Ltd, producer of the Spekker photometer based on photographic detection by means of a quartz spectrograph.

<sup>96</sup> The following relies heavily on the account in Grayson (2004).

<sup>87</sup> *Chemical and Engineering News* (1960), p. 106.

<sup>88</sup> Though space does not permit discussing these texts, the views of Heyrovský & Shikata, (1925), Müller (1946), Ewing (1976) could be adduced as further evidence.

<sup>89</sup> Lewin (1958), p. 21A.

<sup>90</sup> Lewin (1958), p. 20A. My emphasis.

converted into tabular form through a labor-intensive process. The earliest use of computers (1958) in mass spectrometry was that of a digitizer that could tabulate the data as the spectrum was being generated. The Mascot digitizer was itself fairly crude, in that it was unable to do anything else but digitize the output of the spectrometer to which it was hard-wired. But digitization, in turn, enabled new applications of the computer to mass spectrometry in the 1960s. The DENDRAL algorithm was developed to interpret the spectra of unknown compounds, albeit with limited success. High-resolution mass spectrometry, which allows deduction of elemental composition, relied heavily on computers to digitize the data from the detector and process them into exact mass and intensity information. Library search algorithms were developed to match the spectra of unknowns with those of reference compounds. In the 1970s, techniques and instrumentation were developed that allowed the spectrometer to be coupled with a gas chromatograph and a data system. The GC-MS-DS was capable of generating several hundred spectra per half hour, which could eventually (1990s) be compared via library search algorithms to libraries containing hundreds of thousands of reference spectra. In contrast, only a few spectra per hour could be prepared by an operator using a strip chart recording machine of the 1940s and 1950s.

In this section, 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. 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.

Once the new methods were adopted by organic chemists, they supplanted the previous approach of solving chemical analysis problems largely through chemical methods. We are now in a position to see why the common structural properties described in section 4.2 should obtain:

1. In both cases, traditional assumptions about how problems of production should be solved were discarded in favor of a more eclectic approach that draws on diverse fields of science and technology, and in so doing, facilitates the development of methods specially adapted to the given problems.
2. In both cases, the eclectic approach was not simply interdisciplinary. The interdisciplinarity was achieved through the construction of machines that exploited advances in different disciplines and that were used to transform the relevant labor processes.
3. In both cases, since the new methods were based on machines, the ability to engage in the work required significantly more capital than before.
4. In both cases, since the design of the instruments was based on an eclectic approach that itself required dedicated workers, a division of labor arose between specialist instrument-makers and non-specialist instrument users. Automation and black-boxing also facilitated use by non-specialists.
5. In both cases, skills that were crucial for the execution of the production process became marginalized because the new methods made use of different processes than those relevant to the skills.
6. In both cases, machines made automation possible.
7. In both cases, the possibilities for modifying and combining the instruments allowed human cognitive and physical limitations to be circumvented.
8. In both cases, the new methods tended to increase productivity, and given the importance of productivity norms in the societies concerned, this fact was used to motivate their adoption.

## 6. Objections and replies

One of the basic claims of this paper is that a process of transformation of the labor process occurred in chemistry that was not only analogous to mechanization processes in the broader society, but was in part caused by similar factors. A confusing aspect of this episode, however, is that it combines mechanization, a change in the kinds of data produced, and the introduction of the new quantum theory to structural chemistry. This combination gives rise to two related objections:

1. Mechanization involves having a machine carry out a process formerly carried out by a human. This episode is not a case of mechanization, because the data produced by means of the new instruments are radically different from those produced by means of the old instruments.
2. The reconceptualization of chemical structure in terms of quantum mechanics and spectroscopic properties is what drove change in this episode, not the opportunities that mechanization offered for the transformation of labor.

In answer to (1), I reply that mechanization is not incompatible with significant change in the nature of the data. The Instrumental Revolution was a case of what Keating, Limoges and Cambrosio describe as a “creation of an emerging new field of actions between humans and machines and between the humans themselves” (see section 2). The episode resulted in a change in both the object of labor and how operations were performed on it. Before the revolution, the object of labor was the substance whose structure was to be determined. The chemist discovered its chemical properties by deploying his or her (usually his) mental and manual skills on it in a series of laboratory operations. After the revolution, the object of labor is light energy (or the molecule and its fragmentation ions, in the case of mass spectrometry). In order to obtain data, chemists operate machines that, with the aid of instrumentation specialists and (sometimes) technicians, perform a series of operations on the object. Thus the instrumental methods are more machine-centered than classical methods, and their development involved a reconceptualization of the process of compound identification. They also produce a different kind of output, though the final outcome of the compound identification process—the structural representation of the compound—is the same.

The second 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 based on a physical phenomenon. The initial phenomenon, however, was generally useless for other than the physicists interested in the phenomenon itself until the changes described in sections 4 and 5 took place. Mechanization was required to develop methods that had the speed, control, sensitivity and other features needed to produce data informative enough to replace chemical data. Black-boxing, an empirical approach to data interpretation, a new division of labor, and various technical improvements were other elements required to make the methods attractive to ordinary organic chemists.

True, the old methods would never be able to provide certain kinds of structural information, for example on molecular conformation. But there was information loss with the new methods as well. Classical structural chemistry had two principal goals: (1) identify a substance in terms of a structural representation, and (2) learn about the chemical reactions in which the substance participates. Classical methods allowed both goals to be achieved simultaneously. Modern structural chemistry has kept (1) as a goal, but not (2), because the spectroscopic properties that are now employed to achieve (1) are of little chemical interest in themselves.<sup>97</sup> Given the monetary and other costs of

<sup>97</sup> In a 1974 interview, the Nobel laureate Robert Robinson makes the point

adopting instrumental methods, the replacement of chemical methods by instrumental methods would only make sense if goal (2) could be abandoned, downgraded, or replaced by some other goal. In the end, the other goal was synthesis.

A third objection starts from the social class disanalogy mentioned in the last section. Class struggle is central to Marxist theory. But there are no clear analogues to capitalists and workers in the Instrumental Revolution. Therefore, Marx's theory is irrelevant to its analysis. The objection fails, however, because it ignores the equally central role of the labor process in the theory developed in *Capital*. There, it is shown that the characteristics of the instruments of labor, and the structure of the labor process more generally, impose constraints on the application of science and technology to production. I have merely extended this line of analysis to the sphere of scientific production itself.

## 7. Conclusion: The Instrumental Revolution or an instrumental revolution?

In this study, the utility of the analogy with mechanization processes in the Industrial Revolution, as the latter were conceptualized by Marx, has been that it focuses on the cognitive consequences of radical changes in the means of production. These include:

- Changes in the kinds of knowledge and abilities necessary to conduct research.
- Changes in who possesses the different kinds of knowledge.
- Changes in how problems are solved, in the case of mechanization that a larger body of the available knowledge can be applied to problem-solving than would otherwise be possible.
- Changes in the adaptability of the means of problem-solving to specific problems.
- Changes in the relations of epistemic dependence (e.g., in the degree of dependence on external experts, or on semi-skilled technicians).
- Changes in training and education.
- Risks due to lack of understanding of the instruments<sup>98</sup>
- Path-dependence in research due to costs sunk in instrumentation<sup>99</sup>
- Changes in goals due to biases inherent in the new means
- Changes in the role of “specifically” human qualities, like creativity and flexibility, in research<sup>100</sup>
- Questions about which norms are to prevail: scientific (accuracy, reliability, etc.), pragmatic, productivist, pedagogical, etc.
- Changes in the rate of methodological innovation<sup>101</sup>
- Changes in data-to-phenomena reasoning<sup>99</sup>

Previous accounts of the Instrumental Revolution have focused on the question of whether and to what extent the episode fits general models of scientific revolution (especially Kuhn's and Hacking's). This focus is understandable, because the categories employed in these

### (footnote continued)

forcefully that the empirical knowledge of chemical reactions was an independent goal of classical structure determination [Robinson (1976), p. 57]. Professor W. von E. Doering regretted the loss of a “nigh inexhaustible” approach [(2000), v].

<sup>98</sup> In chemistry, Nicolaou & Snyder (2005) claim that excessive faith in instrumental methods sometimes causes chemists to make erroneous structural assignments.

<sup>99</sup> On path-dependence in science, see Peacock (2009).

<sup>100</sup> Perovic (2011) argues that excessive automation of high-energy physics experiments risks missing experimental challenges to the Standard Model of particle physics; Galison (1997), ch. 5 recounts the historical debates over the wisdom of automating HEP.

<sup>101</sup> The impact of the Instrumental Revolution in chemistry on the rate of methods development and on data-to-phenomena reasoning are discussed in chapter 5 of Borg (in preparation). On the impact of the revolution on the reasoning employed in structure determination, see also Seeman (2018).

models are very valuable for bringing out important features of scientific change. Nevertheless, they are not designed to capture the causes and effects brought about by radical changes in the means of production. Because the latter changes can have the consequences listed above, I think it worth considering whether *the* Instrumental Revolution was also *an* instrumental revolution, that is, an instance of a distinct kind of revolution involving radical changes in the means of production. Given the fundamental role of the means of production in the labor process, this kind of revolution is not limited to cases involving mechanization. Nor is it limited to changes in data-producing instruments, but could involve, for example, means of representation or theorizing. The notion of an ‘instrumental revolution’ raises questions for future research. Historically, are there other instances of this kind of revolution in science? Answering this question will involve comparisons across the sciences.<sup>102</sup> Conceptually, what is the nature of such a revolution, considered as a kind of revolution rather than a particular historical episode? As it confronts the Instrumental Revolution, the study of scientific change gains new research questions.

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<sup>102</sup> For example, there is evidence that physiology, astronomy, microphysics and mathematics have undergone something like an ‘instrumental revolution.’ For physiology, see Dierig (2003); for astronomy, see Lankford (1997) and Bigg (2000); for microphysics, see Galison (1997), esp. chapter 5; for mathematics, see Mackenzie (2001).

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