

**Instruments and Domains of Knowledge:
The Case of Nuclear Magnetic Resonance Spectroscopy, 1956-1969**

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Abstract

In this thesis, I traced the development of Nuclear Magnetic Resonance (NMR) Spectroscopy through the pages of the *Journal of Organic Chemistry (JOC)* from the year 1956 to 1969 to understand how organic chemists and Varian Associates—the makers of the first commercial NMR spectrometers—negotiated the identity of the NMR spectrometer. The work of the organic chemists was examined through their publications in the *JOC*. Examining the abstracts from the *JOC* between the years 1956 and 1969 developed an understanding of the ways in which organic chemists used the instrument. To understand the role Varian Associates played in the development of NMR, I examined the company's advertisements in the *JOC*. I traced the changes in advertising style and format in order to see how Varian Associates expected their instruments to be used. I drew three conclusions from this work: 1) organic chemists and Varian Associates together determined what an NMR spectrometer was and how it could be used; 2) the identity of the instrument was negotiated by these two groups, and the novel use of the instrument by the organic chemists and new schemes in advertising on the part of Varian Associates were attempts to shift this identity; 3) NMR spectroscopy was a *domain of knowledge* that was embodied in the NMR spectrometer, and that could only be accessed through the instrument.

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Chapter 1: Introduction

Since their earliest days, chemists have relied upon the proper manipulation of devices, machines, and instruments in order to ply their trade effectively. In this thesis, I explore the development of one particular tool used for chemical analysis—Nuclear Magnetic Resonance (NMR) spectroscopy—between the years 1956 and 1969. Specifically, I will be looking at the introduction of NMR spectroscopy into the field of organic chemistry. Before 1956, NMR spectroscopy was a virtual unknown in the work of organic chemists. Yet, by 1959, books devoted to the topic of NMR spectroscopy's applications to organic chemistry entered a marketplace in dire need for such books. Indeed, the explosion in NMR spectroscopy's applications to organic chemistry came so quickly that D. H. R. Barton, editor of one of these books, commented in his editorial preface:

Prior to 1958, examples of the successful application of nuclear magnetic resonance (n.m.r.) to problems in structural organic chemistry were so few in number that organic chemistry departments could scarcely justify the purchase of expensive high resolution equipment. Now, less than two years later, departments which do not possess an n.m.r. spectrometer are at a considerable disadvantage relative to those where such facilities are available (Jackman 1959, p. ix).

Even Barton, who helped to herald the coming of NMR spectroscopy to organic chemistry, must have been shocked by the rapid acceptance of this new spectroscopic instrument into the organic chemist's lab. Just ten years after writing about the introduction of this new form of instrumental analysis, Barton was again discussing the role of NMR spectrometers in

organic chemistry in the second edition to Jackman's, *Applications of Nuclear Magnetic Resonance Spectroscopy in Organic Chemistry*.

The above Editorial Preface, written for the 1st edition of Professor Jackman's monograph on the *Applications of Nuclear Magnetic Resonance Spectroscopy in Organic Chemistry*, adumbrated clearly the fundamental position that nuclear magnetic resonance was to occupy in organic chemistry. Now, less than ten years later, nuclear magnetic resonance spectroscopy is the single most important physical tool available to the organic chemist. Not only does this technique characterize functional groups, but it describes the relationships of appropriate nuclei to each other in constitutional and stereochemical detail. It is a very powerful method for studying details of conformation in solution. No other method can give such useful detail in the liquid state. Increasingly the method is applied to nuclei other than hydrogen.

During the decade since the 1st edition of this book considerable progress in instrumentation has been made. Spectrometers have become more powerful, more easy to use and, for 60mc/s [megacycles per second] instruments, cheaper. Almost all organic chemistry laboratories now have some sort of spectrometer available (Jackman 1969, p. xvi).

How did this transition—from the virtual non-existence of NMR in the laboratory of the organic chemist to near saturation—occur in a period of time that covered just over ten years? How did NMR spectroscopy become, as Barton describes it, “the single most important physical tool available to the organic chemist”?

Beyond asking questions about the proliferation of NMR spectroscopy within organic chemistry, this thesis will address a number of other issues as well.¹ I will examine

¹ And, certainly, there are more issues that could be addressed than those I have chosen to focus on here. For instance, this case study provides yet another example that runs counter to the commonly held view that developments in science lead to technological innovations. Here it is clear that the work done by the organic chemists was limited by the technological component—the NMR spectrometer. This case also lends itself to the analysis of technological transfers. How did the physicists get organic chemists interested in NMR

the relationship established between organic chemists and Varian Associates—the first makers of NMR spectrometers—to understand how the development of NMR spectroscopy was a cooperative effort. I will then address questions concerned with the identity of the instrument. I will attempt to elucidate the point that changes in the use of the instrument by organic chemists and changes in the advertising scheme of Varian Associates consequentially changed the answer to the question, “What is an NMR spectrometer?” I will close, then with some thoughts about instruments and knowledge production. I will argue that instruments are the physical manifestation of what I call a *domain of knowledge*, and that the instrument both determines the boundaries of the domain while embodying the knowledge—conceptual and material—contained within the boundaries of the domain.² But, before addressing these issues, there are some important background questions that should be addressed.

1.1 What is NMR spectroscopy, and why does it warrant study?

The first question that requires attention before we go any further is, “What is an NMR spectrometer?” The quick and dirty answer is that an NMR spectrometer is an instrument used for chemical identification. But the quick and dirty answer does not truly answer the question, “what is NMR spectroscopy?” NMR spectroscopy means something different to

spectroscopy? While this issue is addressed at least superficially in this thesis, more could be done to explore the transfer between cultures of scientists.

² Here, and throughout, I will be using the definition of knowledge put forth by Michel Foucault in, *The Archaeology of Knowledge* (1972). Here, in speaking about knowledge, Foucault says, “Knowledge is that of which one can speak in a discursive practice, and which is specified by that fact: the domain constituted by the different objects that will or will not acquire a scientific...knowledge is also the space in which the subjects may take up a position and speak of the objects with which he deals in his discourse...knowledge is also the field of coordination and subordination of statements in which concepts appear, and are defined, applied, and transformed...lastly, knowledge is defined by the possibilities of use and appropriation offered by discourse...but there is no knowledge without a particular discursive practice; and any discursive practice may be defined by the knowledge that it forms” (pp. 182-3). I find this language to be particularly helpful in determining the characteristics of the domain (a space for knowledge production) and what is contained within that domain (knowledge in the form or practice, theory, and material).

different people. A quick look inside different textbooks elucidates the point. When teaching undergraduate students in a physical chemistry class about methods used in chemical analysis, NMR is “the study of the properties of molecules containing magnetic nuclei by applying a magnetic field and observing the frequency at which they come into resonance with an oscillating electromagnetic field” (Atkins 1994, p.625). An undergraduate instrumental analysis textbook describes NMR as being “based upon the measurement of absorption of electromagnetic radiation in the radio-frequency region” (Skoog and Leary 1992, p.310). But to the organic chemist, NMR spectroscopy exists as something more than a box with a magnet and radio receiver. To the organic chemist, the NMR spectrometer does more than record the resonance of atomic nuclei. NMR spectroscopy compliments other methods of analysis by “providing a ‘map’ of the carbon-hydrogen framework of an organic molecule” (McMurry 1996, p.454). Thus, organic chemists favor it because it provides not only information about what is *in* the unknown (e.g. functional groups), but also information about the molecular environment. What does that mean? It lets a researcher understand *where* a particular atom (or group of atoms) may be located in relation to other atoms. This feature helps in structure determination—an important component of what organic chemists do (including things like natural product synthesis, medicinal chemistry, and pharmaceuticals, for example).

There is a rich history concerning the development/discovery of NMR. The two men considered to be most responsible for this work—Felix Bloch at Stanford and Edward Purcell at Harvard—shared the Nobel Prize for their efforts in 1952.³ Bloch and some of his physicist colleagues at Stanford exploited the idea of NMR commercially under the aegis

³ For more information on the work of Bloch and Purcell and the creation of nuclear magnetic resonance spectrometers, see for instance Forman (1995), Gerstein (1994), Grant and Harris (1996), Rigden (1986), Shoolery (1995), and Zandvoort (1986).

of the newly formed Varian Associates. Varian's direct marketing of its NMR spectrometers (under the direction of James Shoolery in the Application's Lab) is a significant part of this story, and we will speak more about this in the pages to come. The story of Varian's role in the creation of NMR spectroscopy as a commercial product has been told by Lenoir and Lécuyer in their article, "Instrument Makers and Discipline Builders: The Case of Nuclear Magnetic Resonance" (1995). But where does the study of NMR fit in the broader field of science studies?

The work presented here contributes to current work within the field of science and technology studies in many ways. It situates itself inside of a larger framework that has as its focus the material culture of the laboratory, the interaction that human agents have with that material culture, and issues of knowledge production that occur as a result of those interactions. While this thesis compliments previous works (such as that done by Lenoir and Lécuyer [1995]) it also lays open a number of avenues for further development. A brief review of recent literature in science and technology studies reveals a trend moving towards the investigation of laboratories as sites of knowledge production and instruments as part of a material culture of technoscience.⁴ While many works could be discussed here, two recent books prove exemplary of these types of investigations: Peter Galison's, *Image and Logic: A Material Culture of Microphysics* (1997), and Nicolas Rasmussen's, *Picture Control: The Electron Microscope and the Transformation of Biology in America, 1940-1960* (1997). Both Galison and Rasmussen discuss not only how the introduction of a new instrument affects the development of knowledge within a specific discipline, but also the broader context of how

⁴ The starting point for much of this work has to be Latour and Woolgar (1987). From this point, numerous works have been published discussing the role of experiment, the laboratory, and instruments. While not every work can be mentioned here, I hope this list will give the reader some perspective of how rich and diverse this field is: Ackermann (1985), Callon (1986), Collins (1992), Gooding, Pinch, and Shaffer (1989), Hacking (1983), Galison and Hevly (1992), Knorr-Cetina (1981), Lynch (1982), Pickering (1995), and Shapin and Shaffer (1985).

an instrument must be accepted into the laboratory. The acceptance process involves not only the scientists working within a specified field or discipline, but also a host of other actors—for example corporations, technicians, and funding agencies. To adequately tell the story of the introduction of any new instrument, it is necessary to understand how these groups negotiate with one another. This examination, however, should make clear how the scientists, themselves, took part in this transition. Scientists do not passively accept new instruments into their laboratories. Rather, they take an active part in deciding the nature of the instrument and the consequent altering (or “retooling” as Rasmussen calls it [p. 10]) of their laboratories and their fields of study. Works such as those by Galison and Rasmussen have drawn attention to the complexities involved in the acceptance of new instruments and the sometimes drastic consequences that accepting new instruments have for the transformation of disciplines. In light of this, what can another study hope to accomplish?

In her recent book, *Epistemic Cultures* (1999), Karin Knorr-Cetina examines two separate scientific disciplines: high-energy physics (HEP) and molecular biology. Her ethnographic work draws attention to practices of each group. These practices include not only the methods utilized by each group, but also the material make-up of their respective laboratories—including a discussion of the language of each group, physical space of the laboratory and the instruments it contains. Knorr-Cetina, working from a definition of culture that “refers to the aggregate patterns and dynamics that are on display in expert practice and that vary in different settings of expertise” (8), concludes that HEP and molecular biology are not only separate disciplines, but separate cultures. In separating scientific disciplines in this way, Knorr-Cetina draws attention to the problem of generalizing science studies work. While Galison presents a wonderfully elaborate description of “a material culture of microphysics,” his presentation does not (and cannot according to Knorr-

Cetina) overlap completely with the story told by Rasmussen in his equally well-articulated description of the introduction of the electron microscope into American biology. If this is the case, then it can be assumed that the story of NMR will yield some interesting novelties and that it will contribute to a broader understanding of how the introduction of new instruments into *chemistry* differs from that of other scientific disciplines. While the work of Lenoir and Lécuyer (1995) begins this process, the relation of the instrument maker must be explored with respect to the scientists actively involved in its use—as Galison and Rasmussen have done.

This thesis also moves beyond the work of Galison and Rasmussen by introducing a new dimension into the study of industrial and academic relations—advertisements. While Galison and Rasmussen both include examinations of corporations and scientists in their studies of the multifaceted development and introduction of new instrumentation, they focus most of their attention on the material interactions between these groups. That is, they see the instrument as the primary means of communication. Examination of advertisements, I believe, compliments this by exploring the commercial aspects of the instrument and, thus, the relations between instrument maker and instrument buyer. Because Varian Associates is the sole producer of NMR spectrometers in the time period from 1956 to 1969, the case of NMR presents a unique opportunity to explore how advertisements play a role in shaping the development of a new instrument.

Why the time period 1956-1969?

The first commercially produced NMR spectrometers appeared in 1953. The early instruments were usually individually constructed for a customer. Sales of these instruments

increased steadily during the latter half of the 1950s. In 1961, Varian produced the A-60. The A-60 was the first mass produced NMR spectrometer that incorporated speed, precision, accuracy, affordability, and a convenient size.⁵ Surveying the abstracts from the *Journal of Organic Chemistry (JOC)* draws immediate attention to the effects of the introduction of NMR into the field of organic chemistry. The following charts show the increasing presence of NMR in the chemical literature generally and, more specifically, in the *Journal of Organic Chemistry*.

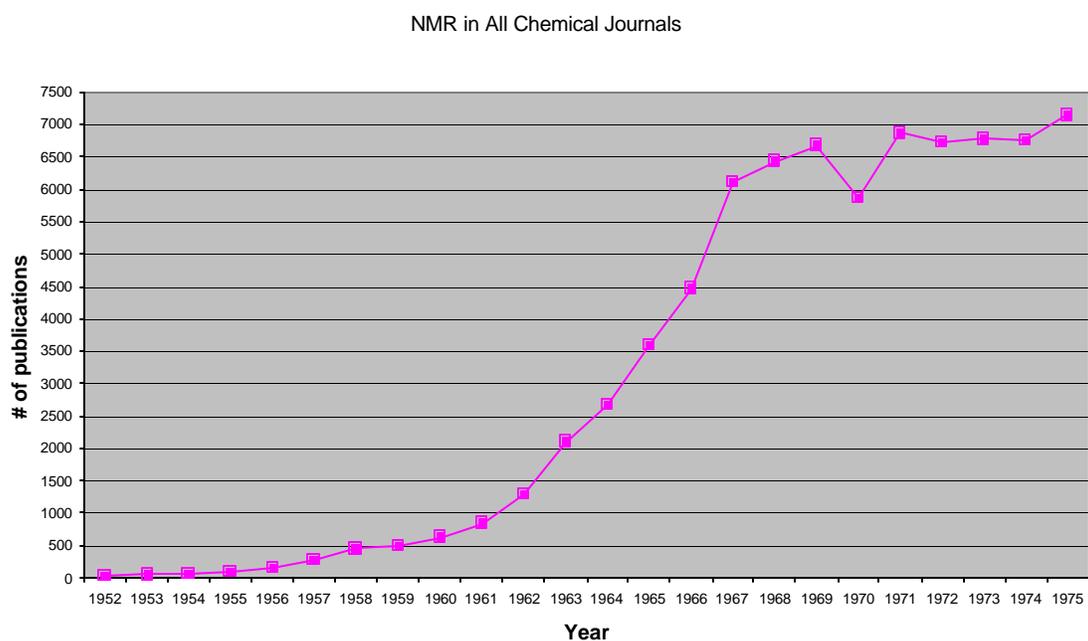


Chart 1. NMR in All Chemical Journals

⁵ It was not, however, the first mass-produced spectrometer. Varian released its HR-30 in 1953, and there were at least four other models released before the introduction of the A-60.

NMR in the *Journal of Organic Chemistry*

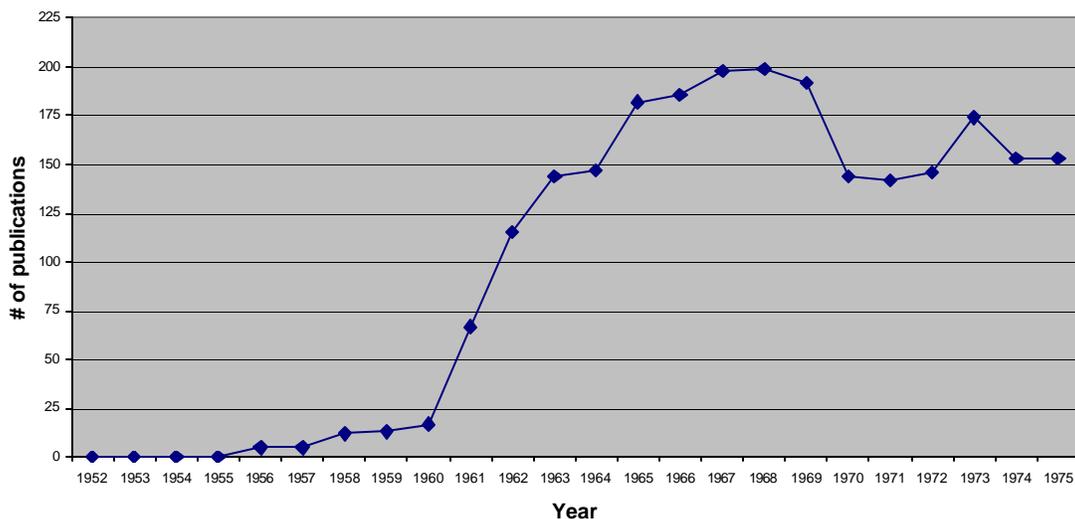


Chart 2. NMR in the *Journal of Organic Chemistry*

The information used for the above charts is based upon SciFinder® search results. Chart 1 refers to the total number of publications between the years 1956 and 1969 that reference NMR in the journals available through the SciFinder database. The second graph looks specifically at the number of publications in the *Journal of Organic Chemistry*.

The graphs help to explain why these particular years were chosen. Before 1956, there is no reference to NMR spectroscopy (at least not in the *JOC*). This trend drastically changes as we enter the 1960s. We also see that following 1969, there is a leveling off of activity. Therefore, the period 1956-1969 encompasses the rise of NMR as a tool for organic chemists and the first plateau of activity.

The years 1956 to 1969 provide bookends not only to the initial work done by chemists and the first plateau of their activity, but also to Varian Associates. Varian ran its first advertisement in the *JOC* in 1958. The company increased the frequency and diversity of these advertisements until 1964, when it had at least one advertisement in 10 of the 12 *JOC* issues published that year. However, following this surge of advertising, Varian quickly

withdrew its NMR advertisements from the *JOC*. By 1967, only one advertisement for an NMR spectrometer appears in the journal. This is the last of Varian's NMR advertisements found in the *JOC* between the years 1956 and 1969. This time period, then, not only encapsulates the first rise in activity of the chemists, but also for Varian Associates.

1.2 The primary players

The story of the development of NMR spectroscopy and its emergence as one of the premier tools within the field of organic chemistry contains many complexities. The story has many players. The players have many goals and there are many obstacles on the way to attaining their goals. To overcome these obstacles, players formed alliances. Here, I will focus on only two of the players and their story in the development of NMR spectroscopy: organic chemists and Varian Associates (the makers of the first NMR spectrometers). For each of these, I will try to define what goals they held, what obstacles stood in the way of those goals, and ultimately how the alliances they formed with one another helped to overcome those obstacles.

Varian Associates

The work of Timothy Lenoir and Christophe Lécuyer (1995) outlines the early history of Varian Associates, its role in the development of the first NMR spectrometers, and the introduction of these instruments into the laboratories of organic chemists. In the coming pages, I will rely heavily on their work when telling the story of Varian Associates.

The initial goal of Varian Associates, as Lenoir and Lécuyer point out, was not to produce of commercially viable products. Instead, the founders of Varian Associates sought

to “create a working environment offering both reliable funding and opportunity to pursue research and development interests in classified military technologies that could not be conducted in an open university environment” (Lenoir and Lécuyer 1995, p.280). Many of Varian’s researchers had spent the war years working on government projects, such as those conducted at the Radio Research Laboratory, and wanted to continue the work that they had begun there. Indeed, Felix Bloch wished to continue his work with nuclear magnetic induction, but initially saw no need to pursue a patent on these devices because he felt it had no commercial value beyond the work of physicists.⁶ By the mid-1950’s, Bloch (working as a consultant to Varian Associates) began to see instrument sales could produce revenue for the company and, thereby, fund his continued research in the field. Indeed, Varian Associates began to explore seriously the commercial possibilities of NMR instruments only after making this connection. Varian now needed to figure out who could benefit from these instruments.

As mentioned above, the unique feature about the information obtained from NMR spectrometers lies within its ability to describe atomic environments. Because the instrument provides information about atomic environments, Bloch and others recognized the potential to detect isotopes in a chemical compound.⁷ It seemed, then, that NMR instruments might have a role to play in the analysis of organic compounds. But how could a group of physicists sell a physics instrument to organic chemists?

⁶ Felix Bloch, working at Stanford, and Edward Purcell, working at Harvard, were the first to report the successful detection of nuclear magnetic resonance in the laboratory (see Bloch et al [1946] and Purcell et al [1946]). In the early years following the initial publications, Bloch refers to his work with the term “induction” while Purcell uses the term “resonance.” While the difference seems to be minimal (from a physicist’s standpoint), the different terms relate how two completely different conceptual frameworks were used to explain what is now regarded as the same phenomenon. For more on the conceptual frameworks used by Bloch and Purcell, see Rigden (1986).

⁷ Lenoir and Lécuyer claim that hints about the instruments ability to do this were already surfacing in 1946, shortly after Bloch’s first publication (1995 pp. 292-3).

The establishment of the Applications Laboratory and the appointment of James Shoolery marked an important commitment on the part of Varian to the further development of a commercial NMR spectrometer for use by organic chemists. Shoolery, who had recently obtained his Ph.D. in chemistry from the California Institute of Technology, realized that before the company could have a commercially viable product, “it was crucial to convince chemists of the indispensability of the technique before a market of research and academic chemists could be created” (Lenoir and Lécuyer 1995, pp. 313-4). The market for chemical instruments was still new, but early work in the development of infrared (IR) spectrometers had created a thriving market.⁸ And since Varian Associates held an exclusive patent on NMR technology, Shoolery knew that he would have to find a way for Varian’s NMR spectrometers to compete with IR instrumentation.

Knowing that he would be competing initially for a share of the IR spectrometer market, Shoolery set out to make the physics of nuclear magnetic resonance comprehensible to chemists. “The goals were to make the results of NMR work interpretable to chemists, to devise new approaches for eliciting information from nuclear radiospectra, and above all to communicate this information to the chemists...[The] immediate obstacles to gaining entry into the chemists’ labs were the cost, size, and unreliability of the instrument” (Lenoir and Lécuyer 1995, p.314). Shoolery, then, was not only interested in making the information that NMR spectrometers could provide invaluable to organic chemists, but also concerned himself with how the information was communicated (i.e. the format), the size and cost of the instrument, and the amount of time a chemist would require to become familiar with the it.

⁸ For one look at the introduction of IR spectroscopy into the field of chemistry, see Rabkin (1987).

These are the issues that I will focus on throughout the examination of Varian's advertising in the *Journal of Organic Chemistry*. I will show that Varian Associates continued to address the issues mentioned above between 1956 and 1969 while responding to the demands and needs of the organic chemists and how Varian shaped the needs and wants of the chemists during this process.

The Organic Chemists

Delimiting Varian Associates and what it does poses few problems, but the same cannot be said for organic chemists. The question, "What is an organic chemist?" contains more complexities than one might think. The term *organic chemist* denotes a wide range of researchers working in vastly different physical and intellectual locations, while the term *organic chemistry* delimits a field of inquiry that contains investigations into anything from the structure of specific enzymes found in metabolic processes to the identification of plant extracts and classification of these compounds based upon their potential for use as medicinal remedies. The *practice* of organic chemistry, too, comes in many forms. Is the organic chemist the one who separates the chemical mixture? Analyzes it using chemical techniques? Analyzes it using physical techniques? Puts the chemicals back together again in a new way? Or discusses the classification of the compounds? The answer is, "it's all of these." The term "organic chemist" does not represent a homogenous group. Nor does the term "organic chemistry" represent a homogenous set of theories, practices, or environments.⁹ While "organic chemistry" can mean many things, it cannot mean *anything*.

⁹ It should be noted that the term "Varian Associates" also does not represent a homogenous group of people or research interests. The development of NMR spectrometers was only one of many projects that the company was involved with during this time period, and certainly not all members of the Applications Laboratory were involved with the same aspects of the project.

Using the term “organic chemistry” implies a certain set of accepted theories, practices, and research agendas. One undergraduate text sums up the definition of organic chemistry quite neatly: “Organic chemistry, then, is the study of organic compounds” (McMurry 1996). While this definition may seem overly simplistic (and perhaps a little misleading), this type of definition serves a purpose. It helps chemists answer questions like, “Where would I go to find information about compound X? Where will I publish my research about compound X? What meetings will I go to talk to others who might be interested in finding out more about compound X? What types of equipment should I use to investigate compound X?” The answers to these questions (and others) define what the term “organic chemistry” means. In this vein, I use the terms *organic chemist* and *organic chemistry* to stand for a certain (although, perhaps, ill-defined) group of chemists involved in chemical research that has been deemed *organic* by the answers that they have provided to the above set of questions. More specifically, I have concentrated upon the *Journal of Organic Chemistry* as a means of delimiting what organic chemistry is as opposed to other types of chemistry.

With that said, organic chemists face certain problems in the course of their work. Some of these problems are unique to their field—others are not. Looking specifically at problems faced by organic chemists in the course of chemical analysis, a number of issues become apparent. When analyzing a new chemical, chemists find themselves constrained by things such as sample size, time of analysis, convenience of analysis, the type of information that can be taken from each technique (and how many different techniques it will take to create a sufficiently complete picture), and the availability of devices necessary for analysis. When we introduce instruments into the picture we also add the problems of instrument size, expense, whether or not the instrument will destroy/alter the sample, ease of operation,

and a host of other concerns. The ideal instrument addresses as many of these issues as possible.¹⁰ It would be fast, easy to operate, inexpensive, take up as little lab space as possible, and provide useful information—consistently. The goal of chapter 2, then, is to understand how organic chemists tried to create this ideal instrument through their use of Varian Associates and its NMR spectrometers.

1.3 Tracking the development of NMR

I have focused most of my attention on the abstracts (plus a few exemplary articles) and advertisements from the *JOC* that reference NMR spectroscopy between 1956 and 1969. With respect to the abstracts, I have traced the uses of the instrument in each of these instances—paying particular attention to “new” or “innovative” uses. For instance, in the first few years covered in this study NMR was mainly used to analyze products of reactions for characterization (much the same way that a chemist would use IR or uv-vis [spectroscopic measurements in the ultraviolet and visible wavelength region] spectroscopy). In the following years, chemists began to explore new areas of organic analysis with the instrument. Chemists used NMR spectrometers for stereo-chemical studies. They used NMR as a quantitative tool. And they discussed how to use NMR more effectively. By examining the abstracts from the *JOC*, I provide a glimpse of what knowledge NMR made available to organic chemists and how this changed during the course of this technological transfer. By looking at the advertisements placed in the journal by Varian, I exhibit what Varian wanted an NMR spectrometer to be—that is, how they wanted it to be used—and how they contributed to the transformation of the instrument.

¹⁰ Naturally, the “ideal” is defined differently for every situation. However, there seem to be certain features that chemists continually searched for in instrumentation.

Relying in this way on only one journal as the primary source for my information has certain benefits.¹¹ By focusing the study on the contents of the *JOC*, I hope to avoid the pitfalls inherent in a broad sweeping study—the creation of a superficial study that fails to elucidate the key points that I make here. I have chosen the *JOC* as my starting point for this study because it represents the most central territory for knowledge in the field of organic chemistry.¹²

This method has also allowed me to become much more familiar with the journal than would have been possible had I chosen to broaden the scope of this project. For instance, I was able to note not only the articles published in each issue, but also the advertisements. One can easily search for the abstracts/articles using any of a number of conventional search engines.¹³ However, one cannot examine the advertisements in a journal without getting *inside* the journal. This allowed me to notice things such as the placement of the advertisements. It gave me a sense of who else was publishing and of Varian's publishing methods compared to other instrument and chemical companies. And it allowed me to get a feel for how the journal as a whole operated.

Just as this method of analysis allows me to see certain things that would have previously remained invisible, the adoption of this line of research also conceals things. First (and perhaps most obvious), by limiting my research to only one journal, I may be placing blinders on myself (or to use a cliché, I may be missing the forest for the trees). What else is

¹¹ I say primary, and not only, because this work is also informed by many of the books that were published at the time in an attempt to introduce organic chemists to NMR studies. See, for instance, Jackman (1959 and 1969), Bhacca (1964), and Carrington and McLachlan (1969).

¹² Certainly, organic chemists read other journals, and people other than organic chemists published in the *JOC*, but the journal embodies a specific field of knowledge. An examination of table 1 above clearly shows that information related to NMR spectroscopy was being published in other areas. However, as has been pointed out to me, the *JOC* is where organic chemists publish their work when they want to speak to other organic chemists. More theoretical work is often published in journals such as the *Journal of the American Chemical Society* (*JACS*), which has a much broader readership.

¹³ For this study, I relied exclusively on SciFinder®, a search engine provided by the American Chemical Society for searching chemical related journals. For more on how this search engine operates, see <http://www.scifinder.com/>.

going on in the world of chemistry? Where else is NMR spectroscopy being used? Are the uses the same? How did outsiders view this new technology? How did the actual technology of the instrument change? What engineering breakthroughs allowed Varian to build different instruments? What did the physicists think about giving NMR spectrometers over to organic chemists? How did the instruments of the physicists differ from those of the chemists? (And on, and on.) All of these are valid questions and *should* be addressed by someone at some point in time. I have chosen to conduct the research in this manner, however, to shed light on issues that often go unnoticed—such as the role that advertisements played in directing this field of inquiry.

An additional concern lies in my reliance upon one database—SciFinder, the online database furnished by the American Chemical Society for searching chemical abstracts—for my information related to the publications in the field of organic chemistry. While I selected this database because I believed it would provide the greatest amount of information from the greatest number of resources, I have also knowingly confined myself to the limits of this technology. The search engine design allows for certain searches, and filters information in a predetermined way. As a simple user of this technology, I have no choice but to submit to these restrictions. While I have done my best to avoid the pitfalls that this imposes, I acknowledge that there may well also be something that I missed.

1.4 Historiographical considerations

In his 1996 article, “Speaking of Annihilation: Mobilizing for War Against Human and Insect Enemies,” Edmund Russell point to two very specific historiographical lessons that bear on our story. The first lesson concerns our tendency to tell one-sided stories:

...We often talk about the impact of one aspect of life (war, science, politics) on another (the state, culture, the environment). This framework tells us a great deal, but is it complete? Few forces are monolithic, and the two-way interactions may be more common than one-way impacts (Russell 1996, p.1510).

I point this out for the following reason. Lenoir and Lécuyer have contributed a great deal about the history and development of NMR spectroscopy from the perspective of Varian Associates. Their detailed analysis of the company's formation and its efforts to create a market for their instruments inside of the chemical arena sheds light on another chapter in the "Big Scientific Instrument Revolution."¹⁴ Indeed, this period of the creation of "big science" has been written on extensively, and Lenoir and Lécuyer's article helps to place chemistry, often times neglected, into the broader picture of American science.¹⁵ What I fear has been lost by focusing on Varian alone in the context of the development of NMR spectroscopy is the role the chemists played in creating and shaping the field. This thesis, therefore, will pick up where Lenoir and Lécuyer left off in their article. I seek to fill in a much-needed piece of the puzzle in the development of what has become "the most valuable spectroscopic technique available to organic chemists" (McMurry 1996, p.454).

Russell's second lesson concerns the language used to describe events in the history of scientific development:

...We may tend to tell stories of progress or decline, but life is a mixture of the two. For some people insecticides and chemical weapons were blessings; for others they were curses; and for some they were both. The world gets both better and worse, and we have yet to exterminate either good or evil (Russell 1996, p.1510).

¹⁴ See for instance Baird (1993)

¹⁵ See for instance, Galison and Hevly (1992) and Galison (1997) for a more focused look at "big science" in physics. For a look at how "big science" affected instruments and biology, see Rasmussen (1997).

Russell's article draws attention to an important problematic in writing the history of technoscience. While scholars within this field have for years argued about historiographical methods, notions of progress still creep into our writings. I have made a conscious effort to avoid any language that implies progress or any other similar concepts. To this end, I will develop the idea of the *domain of knowledge* as a concept outside of this progressive language. The domain evolves, but it does not progress towards an end. The domain shifts as its boundaries are re-negotiated. The domain, then, is my attempt to remove these positivist notions from my historical writings and to overcome the second historiographical issue presented by Russell.

1.5 Disciplines and domains of knowledge

Instruments, like other pieces of equipment, are designed for specific tasks. To perform these tasks, they require knowledge ("thing knowledge" to use Davis Baird's term [Baird, in press]). When organic chemists adopted NMR spectrometers from physicists, they gained access to a certain *domain of knowledge*, but they also entered into the production of that domain. As organic chemists modified the instrument to fit their needs and their interests, and as Varian responded to the work being done by organic chemists in the field, this domain shifted. New questions could be asked of the instrument, and new answers could be expected. This domain, then, is a dynamic network of individual, group, and material agents. Researchers could change it by asking old questions in new ways (thereby "tricking" the instrument into giving information that is not routinely available). Instrument designers, such as Varian, can shift the domain by removing old features and incorporating new features into newer models. More technologically adept researchers may tinker with a

“ready-made” instrument, which can also result in a domain shift. The *domain*, then, is responsive to physical as well as conceptual change.

Domains do not have rigid physical boundaries. Instead, they possess conceptual peripheries that are constantly in flux (constituting a never-ceasing (re/de)territorialization of knowledge, if you will [Deleuze and Guattari 1987]). They constrain us, but only until we find new ways to re-ask, re-design, and re-think the questions and their solutions.

The title of Lenoir and Lécuyer’s 1995 article describes Varian Associates as “Instrument Makers and Discipline Builders.” They claim in their abstract that a certain set of characteristics is required before a discipline can be established. “Crucial to the establishment of a scientific discipline is a body of knowledge organized around a set of instruments, interpretive techniques, and regimes of training in their application” (Lenoir and Lécuyer 1995, p. 276). While I believe this to be true, I do not think it fully represents the formation of a *discipline*. In addition to the aforementioned characteristics (or properties), a discipline must contain a few more crucial elements. Disciplines have independent journals. They have meetings. The members have shared goals. Intellectually, the members demarcate a specialized area of knowledge that they alone can access. And these conceptual boundaries are often manifested in physical boundaries such as separate labs, separate research buildings, with different designs intended to accommodate the specialized needs of those practicing inside of the discipline. While many of these characteristics are, indeed, present in the case of NMR spectroscopy, I believe it is too strong a statement to call this a separate discipline, at least during the time period covered by Lenoir and Lécuyer’s article.¹⁶

¹⁶ NMR studies did eventually obtain their own journal. It is also not outside the realm of possibility that NMR instruments were housed in separate laboratories. However, the term ‘discipline’ seems to me to be applied to cases in which there is a much more substantial break from other disciplines than what we see here. Separate

What, then is NMR spectroscopy? In the time period from 1956 to 1969, NMR spectroscopy constitutes a *domain of knowledge*. The NMR spectrometer provided access to this domain. The use of the spectrometer not only demonstrated the understanding that chemists possessed of the instrument, but also of the knowledge that it provided access to when used. The borders of this domain (and the knowledge found inside of its borders) were in a constant state of negotiation. The contents found within these borders separated NMR spectroscopy from other analytical and instrumental methods.

As mentioned above, I will explore the roles of two players in the creation of these domains in order to elucidate how these domains were constituted and delimited. In chapter 2, we will begin by looking at the organic chemists. We will examine their publications in the *Journal of Organic Chemistry* to see how they used the instrument and how they contributed to the developing definition of what an NMR spectrometer is. Then, in chapter 3, we will look at the role that Varian Associates played in the creation of NMR spectroscopy. We will focus our attention on the advertisements run by Varian in the *JOC* and how they corresponded to the work of the chemists and the development of the company over this 14-year period. I will then close with some remarks about what this study suggests about domains of knowledge.

courses were not offered in NMR spectroscopy to undergraduate students. NMR spectroscopy did not constitute a separate division within the American Chemical Society. And, while separate meetings were being held to discuss the latest in advances in NMR spectroscopy, they were organized by Varian and not by a separate, autonomous group of chemists.

Chapter 2: Abstracts from the *Journal of Organic Chemistry*: The Story of the Organic Chemists

The question, “what is an NMR spectrometer?” invariably entangles itself with the question, “what is an NMR spectrometer used for?” In this section, I will trace the relation between these two questions in the writings of organic chemists and their publications in the *Journal of Organic Chemistry (JOC)* between the years 1956 and 1969. I will begin by maneuvering through the abstracts and occasionally venturing into the technically denser articles that seem to indicate a shift in the use/meaning of NMR spectrometers.

2.1 Structure analysis and determination

The primary use of NMR spectroscopy lies in the realm of structure analysis and determination. Shortly after the announcement of the nuclear magnetic resonance phenomenon, the possible applications to chemistry—and more specifically organic chemistry—began to circulate.¹⁷

Structural analysis and determination dominated the early years of NMR spectroscopy in organic chemistry. The first study to utilize NMR spectroscopy in the *JOC*, entitled “9,10-Dihydro-9,10-methanoanthracene,” was published in 1956 (Vaughn and Yoshimine 1956). The researchers conducting this study—Wyman R. Vaughan and Masao Yoshimine from the University of Michigan—used NMR spectroscopy to confirm the structure of a newly synthesized compound. Other studies conducted that year included the use of an NMR spectrometer to confirm the structure of an organolithium compound

¹⁷ See footnote 5.

(Dixon 1956) and Feist's acid (Bottini and Roberts 1956), and an examination of the nuclear magnetic resonance spectrum of helvolic acid (Allinger 1956).

Understanding *what* organic chemists analyzed in their labs is as important as understanding how they analyzed it. As we see from the few examples mentioned above, the primary use of NMR spectroscopy in the early years was relatively straightforward. Early NMR spectroscopic studies focused on the analysis of newly synthesized organic compounds and the confirmation of structure for previously known compounds. But within one year, organic chemists expanded the use of NMR spectroscopy to analyze steroids (Herzog 1957), deuterated compounds (Bissell 1957),¹⁸ and natural products (Zavarin 1958). These examples were important because they demonstrated the ability of NMR spectroscopy to be used on large, complex molecules. In addition to expanding the use of NMR spectroscopy to larger and more complicated molecules, organic chemists began applying NMR spectroscopy to the study of other atoms within organic compounds.

2.2 Beyond H¹ NMR...expanding NMR to other elements

For NMR spectroscopy to become a truly indispensable tool for organic chemistry, it needed to expand access to knowledge beyond routine proton analysis. In principle, NMR could be used for any element with an odd number of protons. However, organic chemists had interest in only a limited number of elements. The complexity of the analysis increased as chemists sought to analyze more complex molecules. As the desire to analyze a broader range of molecules increased, so did the abilities of the NMR spectrometers.

¹⁸ The deuterated (deuterium is an isotope of hydrogen with two protons instead of one) sample is an exception. It is noteworthy because it demonstrates an understanding of how NMR functions. Deuterated compounds will not resonate like a traditional organic compound, which allows one to investigate certain aspects of the compound while blocking out others.

In 1962, Varian Associates began selling chemists on the use of NMR spectrometers beyond H^1 analysis.¹⁹ Organic chemists responded with papers that demonstrated their ability to use NMR spectrometers in this expanded capacity. The year 1964 saw no fewer than five articles in the *JOC* devoted to the application of NMR spectroscopy beyond traditional H^1 analysis—utilizing both F^{19} and P^{31} resonance frequencies for structural investigations (Solomon and Dee [1964], Newallis and Rumanowski [1964], Logothetis [1964], Mark and van Wazer [1964], and Bose, Das, and Funke [1964]).

The expanded capabilities of Varian's spectrometers—such as the addition of new radio frequency controllers—allowed organic chemists to broaden the research application of NMR instrumentation. Previously “off-limit” structures were now open to investigation. This expansion of application had tremendous benefits for chemists working in fields related to medicinal chemistry, natural product synthesis, and other biologically active compounds. For instance, chemists involved in the synthesis and analysis of steroids used F^{19} investigations in addition to H^1 studies to understand the conformation and three-dimensional structures of these highly complex molecules.²⁰ The development of N^{15} isotope “tracers” allowed chemists to follow conformational changes in complex molecules.²¹ Indeed, the reaction by chemists to these new abilities was so strong that by the end of 1969 at least 59 articles had been published utilizing the expanded capabilities of Varian's spectrometers in the *Journal of Organic Chemistry*.²² The willingness of chemists to apply NMR spectroscopy to new analytical problems prompted Varian to accommodate chemists with new instruments—with more powerful magnets, time averaging computers,

¹⁹ The advertising scheme of Varian is discussed in greater detail in the following chapter.

²⁰ See for example Boswell (1966).

²¹ See for example Lestina, Happ, Maier, and Regan (1968).

²² This represents roughly 5% of all articles referencing NMR between the years 1964 and 1969.

and new radio frequency controllers—while keeping the old instruments from slipping into obsolescence.

With an ever-expanding product line, increased demands from the field of organic chemistry, and an increase in diversity of instrument application, Varian Associates developed the concept of the “Living Instrument”²³ to allow for flexibility in their NMR spectrometers. The “living instrument” constituted a promise on the part of Varian that any previously purchased Varian spectrometer could be modified to perform in the same capacity as any of the new ones being produced. This “upgrade” included not only new features for the spectrometers (such as the C-1024 time averaging computer), but also newer radio-frequency controllers—allowing the chemist to adjust the frequency at which the instrument operated. Since the detection of nuclear magnetic resonance depends upon the ability to replicate the frequency of the target atom, the ability to adjust this frequency is a necessary feature if the investigator wishes to examine multiple target atoms.²⁴ By offering to “retrofit” old instruments with new components, Varian provided researchers who had been involved in the earliest steps of the implementation of NMR spectroscopy to organic chemistry with the ability to continue their work using cutting edge equipment—without have to purchase a new instrument. While chemists explored the ability to expand their structural analyses, Varian was also pushing the application of their instruments beyond qualitative structural analysis and into new territories.

²³ The concept of the “living instrument” is discussed in greater detail in the following chapter.

²⁴In a sense, then, the ability to measure the magnetic resonance of atoms other than hydrogen involved two separate steps. First, researchers needed to determine the frequency for that specific atom. Much of the early work in NMR focused on this pursuit (see for example Bloch [1946], Purcell [1946], and Forman [1995]). The second step involved making an instrument capable of operating at multiple radio frequencies.

2.3 NMR as a quantitative tool

As a qualitative instrument for the analysis of organic bodies, NMR spectrometers were hard to match. They were relatively fast, could operate with small sample sizes, and were non-destructive while delivering a unique data set. As a quantitative instrument, NMR spectrometers offered chemists expanded access to information about sample mixtures and increased problem-solving capabilities through the ability to calculate the percent composition of a sample.

In 1960, Varian Associates ran a series of ads presenting chemists with the quantitative aspect of their NMR spectrometers. Varian ran three ads that year in the *JOC*, and all of them discussed this capability. The ads discussed the instrument's abilities in two ways: as "proton counters" and as a "quantitative analytical technique."²⁵ The following year reflected the success of Varian's advertising campaign. An article by Robert Filler and Saiyid M. Naqvi (1961), described the use of a Varian NMR spectrometer to determine the quantity of a specific compound within a mixture.²⁶ This article was interesting in two respects. First, by demonstrating the instrument's ability to analyze for a specific compound within a mixture, the authors introduced a powerful tool to organic chemistry. Because the instrument could be manipulated to distinguish between multiple compounds, the chemist was freed (in some ways) from having to separate compounds prior to analysis. This was important since separation methods are often long and tedious—and in the worst case they

²⁵ See advertisements in *JOC* v25 issues 4, 7, and 11.

²⁶ I should clarify, perhaps, how this quantitative analysis worked. The analytical output of the NMR spectrometer is a series of peaks (for some examples, see the figures printed in chapter 3). The size of the peaks (or intensity) reflects the relative amount of a certain atom with respect to other atoms (for instance peaks with a ratio of 3:1 represent a 3:1 ratio of those atoms) found in the chemical. Therefore, to conduct a "quantitative" analysis of a mixture of compounds, Varian provided a method for mathematically integrating the peak areas of one compound with the area of another. This information, combined with information about the sample (e.g. concentration of solute in solvent) allows for a "quantitative" determination of the sample.

destroyed the original sample. Removing this step allowed for faster and more diversified analyses.²⁷

The second point of interest lies not in what the article said, but in looking at where the NMR spectral analyses were conducted. The authors of the paper thanked James Shoolery and Le Roy Johnson at Varian for “running and interpreting the NMR spectra” (footnote 5, p. 2572). This occurrence is not unique. Actually, it is far from unique. My point is not to demonstrate unethical tactics on the part of Varian to promote its own equipment by offering to scan samples and interpret data, but to highlight the active role Varian took in supplying organic chemists with instruments for analysis and to make visible the role they (and their associates) played in shaping the field.

Not only did Varian offer its analytical services to chemists,²⁸ many of Varian’s chemists also contributed to the expanding use of NMR spectroscopy in organic chemistry. Most notably, the head of Varian’s Application Lab, James Shoolery, co-authored at least seven papers in the *Journal of Organic Chemistry* between the years 1956 and 1969. Norman Bhacca, another Varian chemist, authored two papers and co-authored at least six more. Bhacca was also in part responsible for the publication of Varian’s two-volume *High Resolution NMR Spectra Catalog* (1962).

In addition to content analysis, chemists also attempted to use NMR spectrometers for additional types of analyses, such as molecular weight determination.²⁹ However, the bulk of the chemists’ quantitative uses for NMR centered on the analysis of chemical

²⁷ This move away from the need for the chemist to separate chemicals before analysis is part of a much broader shift in analytical chemistry following the “Instrument Revolution” in chemistry. Prior to this shift, much of the time analytical chemists spent in the lab revolved around the separation of chemical mixtures. Following the introduction of instruments employing physical methods to analyze mixtures, analytical chemists increasingly moved away from this role of separation artist and became, instead, masters of instrument manipulation. For some discussion on how these changes affected the role of the chemist, see for instance Baird (in press) and Slater (2002).

²⁸ This is discussed further in the following chapter.

²⁹ See for example Barcza (1963).

mixtures, and the determination of the chemical constituents within the mixture. This tool proved particularly useful when dealing with mixtures of stereoisomers³⁰ and assisted in the qualitative structural analysis of these chemicals.

2.4 The complex world of stereochemistry

As chemists' understanding of complex organic molecules such as the alkaloids³¹ grew, organic chemists required an instrument that would help them explore the three-dimensional (stereo) structure of these molecules. Because of the phenomenon that NMR instruments are designed to investigate, these instruments are uniquely suited for these types of investigations. Unlike most spectroscopic instruments, the information provided by NMR spectrometers is not specific to a particular atom's mere presence or the presence of some particular functional group (group of atoms). NMR spectrometers give information about molecular environment. This makes the instrument sensitive to differences in spatial orientation, distance between atoms, and other electronic environmental factors. When manipulated properly, then, the information gleaned from an NMR spectrometer will offer not only a compositional skeleton of the chemical, but also a three dimensional picture of the compound(s).

NMR spectrometers were used for stereochemical analyses nearly from the start. As early as 1961³², organic chemists used the instrument to assign conformational structures and for the analysis of isomeric mixtures. The ability to use NMR spectrometers to investigate

³⁰ McMurray (1996) defines isomers as "compounds that have the same molecular formula but have different structures." That is, they are chemicals with the same atomic makeup, but the atoms are in different relations to one another and a stereoisomer as "isomers that have their atoms connected in the same order but have different three-dimensional arrangements."

³¹ Alkaloids are a class of naturally occurring chemicals (specifically, amines) that normally hold medicinal value; they include morphine codeine, cocaine, and nicotine.

³² See for example Huitric and Carr (1961).

the stereochemistry of a molecule facilitated the application of this technology to fields within (and bordering on) the bounds of organic chemistry.

The search for naturally occurring chemicals with biological activity has long been a pursuit of chemists. Because the shape of a molecule can determine whether or not a chemical will produce certain effects (such as particular biological activities), chemists began to apply NMR spectrometers more frequently to fields such as natural product synthesis, biochemistry, and steroid synthesis. For this reason, the need for conformational—and not just molecular—information related to these products is imperative. There are no fewer than 90 articles devoted to the topics of alkaloid and steroid stereochemistry published in the *Journal of Organic Chemistry* between the years 1956 and 1969. As the capabilities of the instruments changed so, too, did the analysis of these complex molecules. Chemists began to incorporate new features of the spectrometers into their studies. Increased use of F^{19} and P^{31} analyses allowed chemists to increase the scope of their investigations into a broader range of natural products and biologically active molecules. The expansive spectrum of chemicals to which NMR was now being applied demanded an instrument capable of producing spectra more efficiently. One chemical spectrum published in an article was no longer sufficient. If NMR spectrometers were to prove their worth, the chemists had to be able to produce more spectra faster.

2.5 From one sample to one hundred

As NMR spectrometers became more powerful, the speed of analysis also increased. The time for analysis decreased from nearly a day to only minutes. This increase in efficiency led chemists to broaden their investigations from single samples to entire families of compounds. Gone (for the most part) were the days of articles reporting on the NMR

spectrum of a single compound. Instead, entire tables of data were presented. Rapoport and Bordner's 1964 article lists NMR spectra for seven compounds. An article by Subramanian, Emerson and LeBel in 1965 lists 16, and a 1967 article written by House, Latham and Whitesides lists spectral properties for 50 chemicals. What made these dramatic differences possible?

The introduction of Varian's new A-60 NMR spectrometer in 1962 was an attempt to address many of the chemists' concerns and desires for NMR analysis. The A-60's design embodied the key ingredients for any successful instrument—a low price and quick, reliable results. The A-60 did not represent the latest in high-powered NMR spectrometers. Instead, the A-60 (and later the A-60A) embodied Varian's attempts to bring NMR spectroscopy to the masses. While Varian continued to modify and expand its line of spectrometers, the A-60 remained the company's mainstay.³³ The following year, Varian experienced a 65% increase in profits and the number of NMR related publications in the *JOC* increased from 67 in 1961 to 115 in 1962 to 144 in 1963.³⁴

The introduction of new, smaller, easier to operate instruments reinforced other transformations already underway in chemical laboratories. Researchers spent less time running samples and more time analyzing the results taken from instrumental analysis. Instrumental analysis became an everyday procedure usually undertaken by technicians and not chemists themselves. The analysis of organic compounds became mechanized.³⁵ Following the publication of the two-volume *High Resolution NMR Spectra Catalog* by Bhacca et al in 1962, chemists were able to quickly compare their results with the spectra of known compounds. The ability to contribute to this rapidly growing body of knowledge was

³³ In 1963, Varian Associates made 7,734,000 on spectrometer sales. The A-60 accounted for \$3,224,000 of this. See Lenoir and Lécuyer (1995) p. 322, Table 3.

³⁴ See Lenoir (1995) p. 322

³⁵ This issue is discussed again in the next chapter.

facilitated both by changes in the practices of the chemists in their laboratories and also the instruments now made available by Varian.

Chapter 3: Advertisements from the *Journal of Organic Chemistry*:

The Story of Varian Associates

As I mentioned in the introduction, Varian Associates held an exclusive patent on NMR technologies. This fact put Varian in a unique situation. James Shoolery, head of Varian's Applications Laboratory in Palo Alto, CA did not have to worry about competing with other NMR instrument makers. Instead, the marketing and research teams at Varian fought for a share of the broader instrument market. The advertisements of Varian between the years 1956 and 1969 reflect this position. Varian's advertisements did not focus on their instrument's abilities to outperform competitors. Instead, Varian emphasized the indispensability of the information that their instruments could provide. The primary function of the NMR advertisements, then, was to create a sense of necessity for this exclusive information.

3.1 "NMR at Work"

In the early 1950's, Varian began running a series of advertisements known as "NMR at Work." The purpose of the series was to introduce this new analytical tool and the information that it could provide to the world of chemistry.

The "NMR at Work" series first entered the *Journal of Organic Chemistry* in June of 1958 (NMR at Work #48). The title of the advertisement sets the tone for the rest of the page: "Are you missing the information that NMR spectroscopy can furnish?" This first ad proves intriguing on many levels, and we would be wise to spend some time carefully examining this first ad in detail to gain an understanding and appreciation for how these advertisements function. I want to call attention to a few specific aspects of the

advertisement so that we can look to see if and how these change through the years. (See figure 1.) First, note that Varian spells out the meaning of NMR in small type underneath the title. This extra effort on the part of Varian implies that most of the chemists that they find themselves addressing are unfamiliar with the acronym “NMR.”³⁶

Now let us turn our attention back to the title itself in combination with the subtext. Varian wants to emphasize to the practicing organic chemist that their current analytical methods do not provide a complete picture of the sample under investigation. To solve this problem, Varian’s “unique applications laboratory” offers its services. These services come in two different forms. First, the chemists can ask their institutions to purchase an NMR spectrometer for use in his laboratory. However, Varian knows that this option will not be available to all chemists. As an alternative, Varian also hires out its services as an analytical laboratory. These options are further explained in the text on the top right of the advertisement.

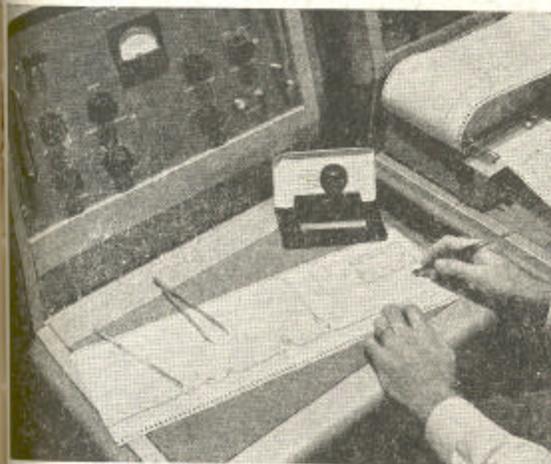
³⁶ As we shall see, this spelling out of the acronym appears in nearly all aspects of our study, but begins to disappear in the mid-1960’s as NMR becomes a more commonplace tool in the organic chemist’s laboratory.

ARE YOU MISSING THE INFORMATION THAT NMR SPECTROSCOPY CAN FURNISH?

(Nuclear Magnetic Resonance)



VARIAN'S UNIQUE APPLICATIONS LABORATORY CAN SUPPLY THESE MISSING DATA



NMR Spectroscopy is a molecular study method that uses a different parameter than any other technique. It can often contribute where other methods are "blind" or inconclusive. Hence NMR may question, confirm or supplement the deductions from your present study methods.

The nuclei H^1 , H^2 , F^{19} , P^{31} and B^{11} yield strong NMR signals that "describe" their molecular surroundings. Thus NMR aids in determining correct structural formulas of such substances as steroids, baranes, natural products and products of organic synthesis. It is useful in studies of molecular conformation, electron distribution in molecules, reaction kinetics, and potential energy barriers in molecules. For example, it determines position and extent of deuterium substitution in organic compounds for study of reaction mechanisms.

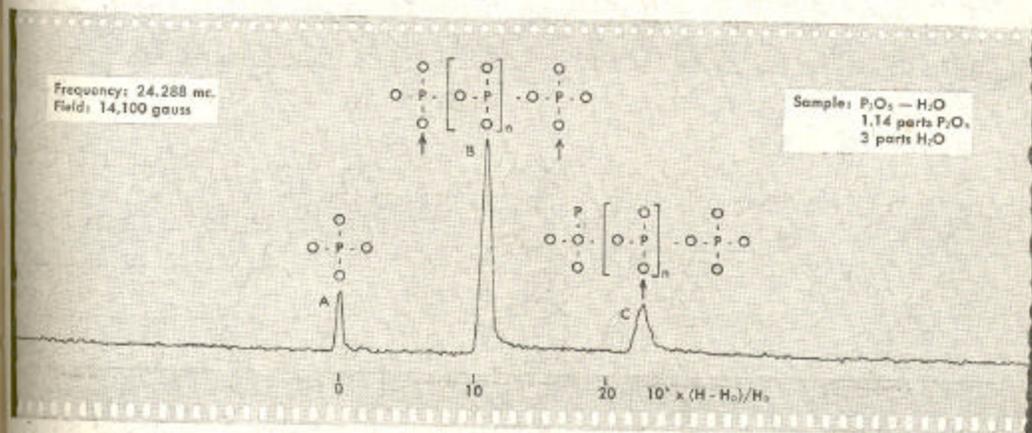
Varian's High Resolution NMR Applications Laboratory has for some time been examining suitably qualified chemical samples on a complimentary exploratory basis. Now in addition Varian will accept a limited number of samples on a fee basis. For \$25 Varian will furnish a brief interpretation and an NMR spectrum taken under standard conditions. More complex studies will sometimes be undertaken on an hourly fee basis.

48 of a series

P^{31} SPECTRA AT 14,100 GAUSS

INTERPRETATION: The analysis of a mixture of ortho-, pyro-, and poly-phosphoric acids is difficult because these species exist in equilibrium with one another. NMR measurements, however, do not shift the equilibrium. The P^{31} resonance is affected by its chemical environment to an extent sufficient to resolve completely the signals from orthophosphate (A), pyrophosphate or polyphosphate end-groups (B), and middle-groups of polyphosphates (C). The areas

under the curves are proportional to the number of phosphorus atoms in each environment. The mixture which gave the spectrum shown below contained an excess of P_2O_5 over the amount required for the formation of H_2PO_4 . The predominant species is pyrophosphoric acid ($N=0$), with a small amount of H_2PO_4 and a larger amount of phosphorus present in polyphosphoric acids.



Selected by the U. S. Government for the Brussels World Fair, Varian 60 mc NMR Spectrometer is available for limited studies while on exhibit.



Write today for additional examples and information on Varian's EPR and NMR Spectrometers and services



VARIAN associates
INSTRUMENT DIVISION

PALO ALTO 25, CALIFORNIA

Figure 1. "NMR at Work" #48

The block of text to the right of the image at the top of the advertisement provides a brief abstract of NMR spectroscopy. The text emphasizes the uniqueness of the instrument and its ability to offer information “where other methods are ‘blind’ or inconclusive” (*JOC* 1958 v23 n6). The advertisement then outlines which atomic nuclei are currently available for analysis and how the signals from these nuclei provide information about the surrounding molecular environment. This information proves particularly potent when studying molecules that have traditionally caused serious analytical problems for the organic chemist—including steroids, boranes, and natural products.³⁷ The information gathered from the NMR spectra—the ad claims—can be used in studies of “molecular conformation, electron distribution in molecules, reaction kinetics...[and] position and extent of deuterium substitution in organic compounds for study of reaction mechanisms.”

The Varian “High Resolution NMR Applications Laboratory” offers its services as an analytical facility for organic chemists who do not have access to an NMR spectrometer. The advertisement notes that the lab has been accepting for some time “suitably qualified chemical samples on a complimentary exploratory basis.”³⁸ In addition to these complimentary services, Varian began accepting samples for analysis at a flat rate, and also offered hourly services for “more complex studies.” Besides *telling* the reader what NMR is and what it does, the advertisement *shows* the reader what an NMR spectrometer can do.

³⁷ The history of organic chemistry is, in a sense, a history of the chemist’s attempts to analyze and characterize many of these molecules. The work done at the end of the 18th century and through the better part of the 19th century proves illustrative of this point. For some examples, see: Brock (1993) pages 173-209, (1997), Roche (1987) and (2000).

³⁸ I think it is important to note this “service” that Varian offered to some chemists. One of Varian’s goals was to compile a “catalog” of spectra that had been scanned on their instruments to be used as a reference tool in the laboratory.

In addition to providing an abstract for what NMR spectroscopy *can* do, the Varian ad offers a specific example of what can be done with their instrument.³⁹ The first example printed here in the *Journal of Organic Chemistry* involves the analysis of a mixture of phosphoric acid. This case proves interesting in two ways. First, the ad exhibits NMR capabilities beyond proton (H^1) spectra.⁴⁰ Second, the example demonstrates how the calculation of area under the curve can yield an analysis that corresponds to relative proportions of product found in the mixture—setting the stage for later quantitative capabilities involving NMR. The “interpretation” discusses the potential problems in analyzing a sample such as this, and then shows how the unique capabilities allow NMR to overcome these obstacles in its analysis.

The effects of the pictorial representation of the sample should not be ignored. James Shoolery, head of Varian’s Applications Laboratory, had the spectral output of the NMR instruments designed specifically to appear like the output from other instruments being used by organic chemists at this time (e.g. infrared [IR] spectrometers).⁴¹ By showing organic chemists what to expect from an NMR spectrometer, Varian accomplished the first step towards establishing their instrument as a new tool for organic analysis—familiarity.

The next “NMR at Work” to show up in the JOC was #58 in the May 1959 issue.⁴²

The advertisement emphasizes the ability of NMR spectrometers to precisely measure

³⁹ Indeed, the entire “NMR at Work” series involves the discussion and resolution of specific problems encountered by chemists in their analytical work. By depicting a specific problem that other analytical techniques could not solve, Varian demonstrated the importance (if not necessity) of using NMR as an analytical tool.

⁴⁰ Because the magnetic resonance phenomenon depends upon the alignment of protons in a magnetic field, only atoms with an odd number of protons can be measured. Naturally, instruments were first designed to measure H^1 in organic compounds. However, the capabilities of the instrument were eventually extended to include other atoms with an odd number of protons—including P^{31} .

⁴¹ See Lenoir and Lécuyer (1995), pp. 320-1.

⁴² It should be noted here that 9 numbers are missing from the series in an 11-month period. It appears as though Varian continued to advertise elsewhere during this time period. However, exploration of where Varian placed those other ads lies outside the bounds of this current project. It is likely that Varian continued to advertise in the *Journal of the American Chemical Society (JACS)*—the journal where the first ads were used.

chemical shifts. The most notable feature of the ad is located in the example spectra. The example itself does not appear to be anything special—“Structure of Photo-Gamma-Tropolone Methyl Ether.” However, the source of the example presents a new feature from not found in #48. Varian did not supply the example. Instead, Dr. Orville L. Chapman from Iowa State College’s Department of Chemistry provided the sample problem and “interpretation.” This use of examples provided by outside chemists seems noteworthy for several reasons. First, if organic chemists can provide examples for publication in an advertising series, then it seems safe to assume that organic chemists have access to the instrument. This does not necessarily mean that they, themselves, have an NMR spectrometer in their lab, but that they have access to one.⁴³ As we shall see, the use of examples provided by chemists outside of Varian becomes a common feature of the “NMR at Work” series.

While one cannot deny the importance of the issue of access represented by outside contributions, it is perhaps more important that Varian was able to convert the “NMR at Work” series into a forum for practicing chemists—a space for new examples to be presented and (eventually) for discussion of those examples. This series provided a space where new information was communicated and examples furnished for later comparison. In this sense, the advertisement itself has become a journal article—something that organic chemists could look forward to reading so that they could stay up to date on the latest developments in the abilities and techniques for resolving specific analytical problems—

⁴³ This access could come in different forms. If the chemist does not have one immediately available in the lab, perhaps a nearby institution has one. Or, perhaps the chemist knows someone who does have access to the instrument. Finally, as we noted above, Varian’s Applications Laboratory offered its analytical services to the academic public for a small fee (although, this seems unlikely in this case since the Applications Lab also provided an interpretation of the sample—something that Varian, here, thanks Dr. Chapman for doing).

problems that many of them encountered on a daily basis, themselves. In short, Varian created a journal inside of a journal.⁴⁴

Although the characteristics of the advertisements remained nearly constant over the next few years, the frequency with which the ads appeared in the *JOC* increased to nearly one in every other issue. Topics normally fell into the categories of possible uses listed in the first ad (*JOC* 1958 v23 n6, discussed above)—for example, a study of the “Location of Deuterium in Anisole – d₃” (*JOC* 1959 v24 n7).

In 1960, the advertisements were reformatted. The headlines began to focus more on specific categories of questions rather than as a general introduction to the instrument itself. The full name behind the acronym for NMR could still be found spelled out underneath in small print, but the ad seemed to imply a familiarity that earlier ads lacked. Themes presented in 1960 include “How NMR Spectroscopy Determines Molecular Structure,” (with an example of how to distinguish between an amine and an imine⁴⁵) and “Proton Counting in Complex Molecules by NMR Spectroscopy,” but most importantly the last two ads published in 1960 introduced NMR spectrometers into a new area of chemical

⁴⁴ Unfortunately, I cannot explore this point further in this project. It would be fascinating, however, to explore the relationship between the “NMR at Work” series and the founding of the first journals devoted to NMR studies. Perhaps this could help to explain the sudden and dramatic withdrawal of the series from the *JOC* in 1967.

⁴⁵ An amine, according to McMurray (1996), is “a compound containing one or more organic substituents bonded to a nitrogen atom,” while an imine is an amine that has formed a double bond to an organic substituent.

analysis—as quantitative tools.⁴⁶ The advertisements read, “NMR Spectroscopy is now a Quantitative Analytical Technique, “ (*JOC* 1960 v25 n7 and 11).⁴⁷

Recall that Varian Associates’ first advertisement in the *JOC* (*JOC* 1958 v23 n6) alluded to the use of NMR spectrometers as quantitative tools. By 1960, Varian provided two examples, the analysis of reaction mixtures (*JOC* 1960 v25 n7) and the determination of C¹³ enrichment (*JOC* 1960 v25 n11).⁴⁸ The advertisements, as usual, provided a detailed description of how the sample was analyzed and how the final values were calculated. The benefits to this method over other types of quantitative analysis included the instrument’s speed and, more importantly, the claim that the analysis took place “without altering or destroying” the sample. This feature allowed the sample to be recovered following analysis in its original form—something that other methods could not do. Again, the choice of examples proved to be interesting. Chemists routinely analyzed mixtures to determine a ratio of isomers, and the study of C¹³ enrichment continued to expand the use of the NMR spectrometer beyond simple proton analysis.

There is an important conceptual feature found in these advertisements as well. In their book, *Leviathan and the Air-Pump* (1985), Shapin and Schaffer discuss the idea of “virtual witnessing.” They argue that, “the technology of virtual witnessing involves the production in a *reader’s* mind of such an image of an experimental scene as obviates the necessity for

⁴⁶ The description that accompanies this ad states that the ability to “count protons” is better than traditional calculations because those traditional methods were only useful with small molecules that contained few hydrogen atoms. The problem of size in structural determination in analysis had long been a thorn in the side of organic chemistry. Attempts to find more accurate methods for the analysis of large molecular weight samples dates back at least to the early 19th century when the alkaloids became a proving ground for new methods of analysis. It was in this vein that Justus von Liebig designed his now famous kaliapparat. For more on this, see Brock (1997) and Rocke (2000).

⁴⁷ An interesting note to this is that the ability to count protons is what makes the NMR spectrometer quantitative. However, Varian Associates seemingly thought that they needed to be more explicit in their advertising.

⁴⁸ The “analysis of reaction mixtures” is noteworthy for its quantitative implications as well as its demonstration that NMR spectrometers remove the need for chemists to separate mixtures of samples before analysis.

either direct witness or replication” (p. 60). The technologies that Shapin and Schaffer refer to involved “linguistic resources” as well as visual representations (pp. 60-1). That is to say, the experiment was recreated within the text through words and images to provide the readers with the opportunity to “witness” the experiment. How does this coincide with what we have seen in the advertisements published by Varian?

As noted earlier, the style of Varian’s “NMR at Work” series had created a “journal within a journal.” Shapin and Schaffer call attention to the need to rethink what a scientific text is: “We usually think of an experimental report as a narration of some prior visual experience: it points to sensory experiences that lie behind the text. This is correct. However, we should also appreciate that the text itself constitutes a visual source” (p. 61). This makes sense in the context of the Varian advertisements. In the earlier examination of the first “NMR at Work” to appear in the *JOC*, it was clear that Varian took great pains to detail the information made available through the use of their spectrometers and to *show* organic chemists what that information looked like. They not only describe the analysis of a mixture of phosphoric acid, the researchers show you the same spectra that they saw during the analysis. The researchers in the Applications Laboratory were welcoming organic chemists into their laboratory to demonstrate the capabilities of NMR spectroscopy.

The following year’s two ads saw a repeat of themes from the previous year. Again, Varian touted the spectrometer’s ability to count protons in complex molecules and offered another example of how NMR determines molecular structure. Interestingly, the ad explaining how NMR determines structure used nucleosides⁴⁹ as the example (*JOC* 1961 v26 n7). John S. Webb, working at Lederle Laboratories, submitted the sample to Varian for use. This example demonstrates two things. NMR spectroscopy is being used for the elucidation

⁴⁹ The study of nucleosides is directly tied to DNA studies. It could be that this move may mark a shift within the fields of biochemistry or biology into DNA and RNA synthesis or other related fields.

of complex molecular structures. And, NMR can offer assistance in fields extending outside of organic chemistry—namely biochemistry.

The Varian advertisements were again redesigned in 1962. Although issues 1 and 5 of the *Journal of Organic Chemistry* contain ads with familiar themes—“NMR Spectroscopy is now a quantitative Analytical Technique” and “How NMR Spectroscopy Determines Molecular Structure”—new ads accompanied the release of the company’s new HR-100.⁵⁰ Two of the five advertisements published in 1962 have “NMR Studies at 100 mc [megacycles]” as their subjects (*JOC* 1962 v27 n4 and 12). The new instrument, claimed Varian, was “the most powerful research instrument available in the field of NMR spectroscopy...solving many problems where overlapping signals previously created ambiguities” (*JOC* v 27 n4 and 12). Greater resolution on the part of the instrument allowed researchers to elucidate more complex molecular structures and opened up the possibility for quantitative analysis where previously this would not have been possible.

Varian also increased its emphasis on NMR spectrometers’ ability to work on samples beyond simple proton analysis. In the September issue of the *JOC*, Varian ran an ad that demonstrated the ability of NMR to analyze F¹⁹ in a sample. To do this, Varian includes an additional RF (radio frequency) unit capable of oscillating in a range compatible with fluorine. Other units available for purchase included RF oscillators for the detection of B¹¹, C¹³, N¹⁴, and P³¹ for more specialized analytical needs.⁵¹

I should note one final observation about the advertisements found in the *JOC* in 1962. So far we have been tracing the Varian “NMR at Work” series. I began in 1958 with

⁵⁰ The HR-100 was actually developed in 1959, but references to its capabilities do not appear until 1962. I assume that this lag in time represents when the instrument was first developed at Varian versus when it was released commercially.

⁵¹ The ability to update and modify the instrument to suit a particular lab’s needs becomes a more prominent piece in later Varian advertisements.

#48. Since then, the frequency of the series in the pages of the *JOC* has increased significantly—from one in 1958 to five in 1962 (an ad in almost every other issue). From the number in the series, it can be assumed that the ads were being placed in other journals as well. We've already noted that the ads first appeared elsewhere in the chemical literature. However, the year 1962 saw five consecutive ads published in the *JOC*—beginning with #78 and ending with #82. It appears that Varian had shifted its full focus onto the readers of the *JOC*.

Together with 1962, 1963 saw the heaviest concentration (5) of Varian's "NMR at Work" series in the *Journal of Organic Chemistry* to date. The ads focus on themes directly related to the HR-100, "NMR Studies at 100 mc" and "NMR studies at 23,500 Gauss." The examples for the first set all focus on the use of NMR to clarify previously ambiguous samples. Comparisons between the spectrum of a sample at 60-mc versus the spectrum at 100-mc presented pictorially allow the reader to literally *see* the difference in instrument capability. Examples for the latter set again include analysis of fluorine and introduce an analysis of phosphorous. Despite the repetition of previous themes, Varian did not limit their advertising to the "NMR at Work" series.

3.2 Moving beyond the "NMR at Work" series

In addition to the "NMR at Work" series, Varian Associates also introduced a new set of publications into the *JOC*—the "NMR/EPR⁵² Spectroscopy Instrument Information Memo" (*JOC* 1963 v28 n7) (See figure 2.) The memo format provides Varian with an opportunity to address in greater detail the specifics concerning their instruments, their use, why a chemist needs one, how to get one, and how to get access to one of Varian's if the

⁵² Electron paramagnetic resonance (EPR), roughly put, highlights the same physical phenomenon as NMR except that it focuses upon electrons in a magnetic field rather than protons.

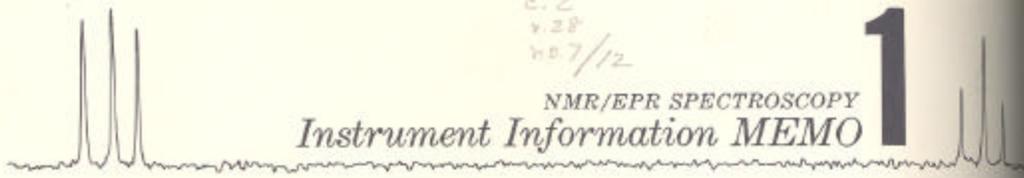
chemist can't get one. Not surprisingly, the first piece in this particular memo compares 60-mc operation with 100-mc operation. The piece outlines the heightened abilities of the new HR-100 in structure elucidation. Varian also announced the opening of two additional Applications Laboratories away from the original location in Palo Alto: one in Pittsburgh, Pennsylvania and the other in Zug, Switzerland. Researchers with analysis problems are encouraged to schedule an appointment to meet with a Varian applications chemist at one of the three sites so that they can tackle the problem together using the latest in NMR technology. The piece also addresses advances in the ability for NMR spectrometers to "decouple" protons⁵³ in samples using a radio frequency oscillator. Of more interest, however, is the introduction of Varian's "living instruments."

⁵³ The process of "decoupling a proton" involves manipulating the radio frequency range emitted by the instrument so that "splitting" (that is the appearance of multiple peaks where there should be only one) is minimized.

QD241
J6
c.2
v.28
no.7/12

1

NMR/EPR SPECTROSCOPY Instrument Information MEMO



ANALYTICAL INSTRUMENTS  VARIAN associates

A COMPARISON OF 100-MC AND 60-MC OPERATION

The enhanced chemical shift to spin coupling ratio provided by 100-Mc operation has helped resolve several structure problems where overlapping lines or multiplets resulted in an impossible or questionable interpretation at 60 Mc. In addition, mixture analyses are usually simplified, since the enhanced shifts often permit identification of resonance lines unique to individual components of the mixture.

We believe that any laboratory with organic structure problems should consider NMR operation at 100 Mc. The enhanced sensitivity, combined with the Varian Microcell, now allows excellent spectra to be obtained from as little as one micromol of sample. The improved signal-to-noise also permits more accurate quantitative results when integrating spectra from samples that had "borderline" signal-to-noise at 60 Mc.

Although the HR-100 has been used to solve a number of problems, some of which have been published in the "NMR at Work" series, we realize that reading about someone else's problem is no substitute for tackling your own problem on a 100 Mc instrument. Similarly, it is impossible to evaluate the performance and capabilities of an instrument on the basis of published specifications alone.

Because of this, we have established laboratories in Pittsburgh, Pennsylvania; Zurich, Switzerland; and Palo Alto, California, where you can bring your problem and work in collaboration with our applications chemists. Please write for an appointment and briefly describe your problem. See "NMR at Work" Nos. 79, 82, 83, 84, 85.

PROTON-PROTON DECOUPLING

A great deal of interest has been generated in the last two years relative to spin-spin decoupling of like nuclei. Various modulation schemes have been used with success. Since the Varian V-3521 electronic integrator utilizes a modulation frequency of two kilocycles for the purpose of baseline stabilization, it seemed only logical to make use of this system for spin decoupling.

Fortunately, by a change in the index of modulation and the use of a variable frequency audio oscillator, the V-3521 becomes not only a precise integrator, but a versatile spin decoupler for like nuclei decoupling. The proper index of modulation was achieved by inserting a 0.01 μ fd capacitor in the modulation leads to the probe. The new V-3521A, supplied as a standard item with all HR-60, DP-60, and HR-100 systems, is now used as both a spin decoupler and an integrator. Details of the modification and the decoupling operating procedure are available in the latest *Varian Technical Information Bulletin*, Volume III—Number 3.

Although work done to date has been primarily concerned with proton-proton decoupling, there is no fundamental reason why the V-3521A cannot be used to de-



Varian's newest Applications Laboratory is located at Pittsburgh, Pennsylvania.

couple Pⁿ, P^m and Fⁿ, F^m spin-spin couplings, provided the chemical shifts observed are not equal to, or some multiple of, the modulation frequency which was initially two kilocycles.

"LIVING" INSTRUMENTS

Throughout its history, the Varian Analytical Instruments Division has maintained a policy of supplying research analytical chemists with "living" instruments. This policy has required a basic activity:

1. The maintenance of a laboratory staffed by research and application chemists who work in various areas of chemistry. Their responsibilities include independent research, collaborative research on problems presented by scientists outside the company, the evaluation of newly designed instruments from the viewpoint of a working chemist trying to solve his problems.
2. The design of new instruments and accessories compatible with instruments presently installed in various laboratories throughout the world.

As a result of this policy, we have been able to offer accessories or conversions to convert older systems to the latest specifications with each new advance in the fields of NMR or EPR. For example, our NMR systems operating at 30, 40, or 60 Mc may be converted to 100-Mc systems with the same performance specifications as our new HR-100, the most powerful NMR research system available.

For additional information write to the latest *Varian Technical Information Bulletin*, Volume III—Number 3, and request the "NMR at Work" series.

For more information about Varian NMR and EPR systems, write the Analytical Instruments Group, Varian Associates Instrument Division. In Europe contact Varian A. G., Zug, Switzerland.



Figure 2. "Instrument Information Memo" #1

In the last piece found in the first memo, Varian describes their instruments as “living.” The concept of a living instrument is meant to imply the versatility and adaptability of the instrument to new tasks and new technologies. The Applications Lab is charged with maintaining this vitality; specifically their activity centers on:

1. The maintenance of a laboratory staffed by research and applications chemists who work in various areas of chemistry. Their responsibilities include independent research, collaborative research on problems presented by scientists outside the company and the evaluation of newly designed instruments *from the viewpoint of a working chemist trying to solve real problems.*
2. The design of new instruments and accessories *compatible with instruments presently installed* in customer laboratories throughout the world. (*JOC* 1963 v28 n7)

Put simply, the job of the Applications Lab is to remain active in the field and to design instruments accordingly. Additionally, current customers should not have to purchase a new instrument every time Varian develops a newer model. Instead, every model should hold the potential for upgrading. The piece specifically points out that an NMR spectrometer “operating at 30, 40, or 60 Mc may be converted to 100-Mc operation with the same performance specifications as our new HR-100” (*JOC* 1963 v28 n7). For more information, readers are pointed towards the “NMR at Work” series.

Varian's "Instrument Information Memo 2" also appeared in the *JOC* in 1963 (*JOC* v28 n10). The second memo announces a new device that regulates the magnetic field inside the NMR spectrometer. In accordance with Varian's concept of the "living instrument," the new device can be exchanged for the old regulation device in previous instruments. The introduction of the "Instrument Information Memo" appears significant. The "ad" functions as such, but much more. The memo takes the form of both brochure and technical paper. Specifics of the instrument can be found as well as contact information, but the memo also contains a hint of journal style writing. While not offering the same straightforward analytical examples as the "NMR at Work" pieces, the memo still addresses laboratory concerns from the perspective of the researcher. This complimentary piece to the "NMR at Work" series moves more towards traditional advertising while attempting to remain technical in style and content.

The year 1964 saw a marketing blitz on the part of Varian Associates. The company missed only two issues of the *JOC* (June and December) using everything it had in its arsenal. The "NMR at Work" series appeared five times (#88-92 in n2, 4, 5, 8, and 10), the "Instrument Information Memo" returned for four visits (#3-6 in n1, 3, 7, and 9). In addition, Varian resorted to more traditional advertising on two occasions (n5 and 11). While the "NMR at Work" series continues to expound upon the power behind the new HR-100, a move back towards some earlier themes is also evident.

The "NMR at Work" series featured only one application example of the (now not so) new HR-100. Instead, two of the five focus on studies that can be done at 60 mc and two others return to explaining "How NMR Spectroscopy Determines Molecular Structure." This return to explaining the basic functioning of NMR comes after a year of

decreased sales profits.⁵⁴ Perhaps Varian felt that they were losing ground with their basic operations while they had been focusing intently upon the sale of their higher-end equipment. The most important feature of this series occurs in nos. 91 and 92. In no. 91, the example focuses on “a choice of two isomers.” Two isomeric structures are given and the NMR spectrum analyzed. Based on the spectrum, the analysts at Varian concluded that structure B seemed more favorable than structure A. However, “NMR at Work” no. 92 revisited the issue of these two isomeric forms. John D. Roberts, a professor at the California Institute of Technology, wrote to Varian and said that the NMR spectrum combined with information taken from a mass spectrometer indicated a third, more probable, option. The authors of the series at Varian discussed the finding reported by Roberts and explained how the third option seemed to accommodate the information better than the previous attempts. I point this episode out not because Varian made a mistake in their analytical lab, but because this exchange demonstrated the advertisements’ function as a legitimate source of information. Varian submitted analytical results to the broader community.⁵⁵ In this instance, the community reviewed the results, studied the interpretations offered, and decided that an alternative interpretation—based upon more data—presented a more likely case. Varian responded by explaining their previous position, presenting the new information, and discussing how one might have read the data the way they had originally. Additionally, no. 92 also cites works by Roberts and others and supports these new findings with reference to previously known spectra found in the *Varian NMR Spectra Catalog*. This exchange seemed to exemplify Varian’s first goal of the Analytical Instruments Division (quoted above), which charges the lab with engaging in dialogue with

⁵⁴ See the chart in Lenoir and Lécuyer (1995) p. 304.

⁵⁵ There is, of course, an obvious difference here. Varian pays for their space, and others are granted this space after intense peer review.

the scientific community. It also speaks to the idea of “virtual witnessing” discussed above. Indeed, the advertisement recreated the experimental atmosphere enough that discussion with outside researchers resulted in a reevaluation of the “results.” It just so happens that this dialogue took place through the medium of an advertisement.

The “Instrument Information Memo” series continued to straddle the ground between brochure and technical information bulletin (although in many ways the brochure side became more prominent). Much of the space of the four memos was devoted to the discussion of instrument upgrades available to current NMR spectrometer owners. Additionally, Varian used the space to discuss new instruments (such as the HA-60, DA-60, and HA-100), the availability of solvents, the second volume of the *Varian NMR Spectra Catalog* a series of NMR workshops to be held at the two U.S. Applications Lab sites, and the announcement of Varian’s 8th Annual Conference on NMR and EPR. From the technical standpoint, the memos continued to address the use of time averaging to eliminate (or significantly decrease) background “noise”—especially when a researcher purchased the Varian C-1024 Time Averaging Computer for use with a Varian spectrometer.

In addition to the “NMR at Work” series and the “Instrument Information Memo,” Varian also began to engage in more conventional forms of advertising. The first of two such ads focused again on the topic of improved sensitivity through the use of the C-1024 Time Averaging Computer. The second ad announced the release of three new instruments—the HA-100, HA-60, and DA-60. The new instruments incorporate many of the features recently developed by Varian for increased performance—including the C-1024. As noted previously, Varian pushed the concept of the “living instrument.” All of the new instruments were compatible with Varian accessories. Additionally, old instruments could be made to perform at the same level as these new ones. These common themes found in the

Varian advertisements were a result of careful planning and high repetition. After two years of an almost constant presence in the *JOC*, Varian had created the market base that it needed. The marketing blitz that took place in 1964, however, gave way to a new style of advertising for Varian.

While the nearly constant presence of Varian Associates remained in the *Journal of Organic Chemistry*, many of the familiar features of Varian's advertising campaign had begun to fade away. In 1965, Varian ran only two ads from the "NMR at Work" series (nos. 93 and 94). Both ads focused on further uses for the 100-mc instruments. In place of the "NMR at Work" series and the "Instrument Information Memo," Varian resorted to a more conventional approach to advertising.

3.3 Getting back to basics

While continuing to advertise for its newest models (the HA-100, HA-60, and DA-60), Varian reintroduced a favorite into the market—the A-60.⁵⁶ Two ads informed chemists that "Now's the Time to Reconsider NMR." Why? Increased signal resolution from the addition of the C-1024 Time Averaging Computer had eliminated noise and made results more clear. Varian's marketing of the A-60, however, did not end there.

In the May issue of the *JOC*, Varian Associates introduced an updated version of the A-60, the A-60A. The advertisement for the new A-60A had much to say—textually and pictorially. (See figure 3.)

⁵⁶ Every chemist I have spoken with about the early NMR spectrometers seems to glow when I mention the A-60. For those that were around during its introduction, they recall the instrument as if it were a beloved friend. Clearly, this is what Varian intended when they designed the instrument. Although it is not the fastest or most powerful of the early spectrometers, the A-60 was designed to be a cheap and reliable instrument—a workhorse for the everyday organic chemist.

This is not our A-60 NMR spectrometer



This is our more sensitive, stable, reliable NEW A-60A

It looks a lot like the A-60, but only until you turn it on. Then you find out about the sensitivity . . . 12 to 1. In fact, you may find the A-60A's high sensitivity and stability now makes NMR practical for your applications.

Send for our new A-60A brochure. It tells all about the improved recorder, slower sweeps, smaller sample concentrations, and shorter warm-up periods. It also explains why the A-60A is insensitive to its magnetic and temperature environment.

Two more things you'll like: The A-60A is so stable that resolution will hold day after day without retuning; and you don't have to double-check single scans. The A-60A gives you stability never before available in a routine NMR system. When you get right down to it, the price is just about the only thing that hasn't changed.

 **VARIAN ASSOCIATES** ANALYTICAL INSTRUMENT DIVISION
PALO ALTO 25, CAL. • ZUG, SWITZERLAND

Figure 3. "This is not our A-60 NMR spectrometer"

For the chemist who already used the A-60, external features of the design had not been changed, inducing a sense of comfort and familiarity. For those who had been either frustrated with certain drawbacks of the A-60, or reluctant to purchase the original, Varian described the improvements built into the new model. Sensitivity had been increased. The instrument could operate with smaller sample concentrations. And, perhaps most importantly, the new A-60A was unaffected by the magnetic and temperature environment of the lab. Varian then added, “Two more things you’ll like” (*JOC* 1965 v30 n5). The first feature allows the instrument to operate for days without tuning. The second ensures an accurate scan that doesn’t need someone to double-check it. These features were important because by removing the need for constant retuning and ensuring confidence in the first scan, Varian was making NMR accessible to a wider audience. A laboratory would not need to employ a specialist just to run and read NMR samples. Instead, vast amounts of data could be collected and processed by technicians who then passed along important and exceptional data to the laboratory chemist. The picture that accompanies the ad reemphasizes this move towards routine NMR spectroscopy.

Additional features also stick out from the advertisement for the A-60A, including: the size of the instrument with respect to the operator. Early NMR spectrometers were enormous instruments. Most laboratories simply could not accommodate one. The magnets were so large and so heavy that the physical structure of the laboratory often times had to be reinforced. Varian had made it one of its primary goals to overcome these physical restrictions, and the A-60A did just that. From the picture, one can judge the relative size of the instrument and the operator. The instrument was more than compact; the NMR spectrometer was no bigger than a work desk and could easily be accommodated

to many laboratory environments. It became possible to place an NMR spectrometer in the laboratory without having to displace other instruments. The operator, then, became more efficient at running multiple tests without leaving the lab.

In the January issue of the *JOC*, Varian again ran its ad for the new A-60A NMR Spectrometer. While this was not the only ad Varian ran in the 1966 volume of the *JOC*, it was the only ad for their NMR spectrometers. Instead, Varian focused this year on marketing their new mass spectrometer to organic chemists. Three ads for their mass spec appeared in the journal's pages, and while a new era was beginning for Varian, another was quietly fading away.

3.4 The end of an era (?)

The last of the “NMR at Work” series to appear in the *JOC* did so in the November issue of 1966.⁵⁷ While brandishing a new design, no. 97 discussed further studies conducted at 100 MHz using C^{13} NMR spectroscopy. The number in the series, however, is, itself, noteworthy. The publications in 1965 concluded with no. 94 in the series. For four years, the *JOC* contained the entire set of the “NMR at Work” series. This marketing strategy on the part of Varian had now changed.

Varian's final advertisement for NMR spectrometers appeared in the *JOC*'s March issue in 1967. The ad depicts the A-60A with its “standard accessories.” (See figure 4.) In keeping with its original mission as both an instrument manufacturer and a research facility, Varian continued to sell itself (and its employees) along with the instruments. Varian was done advertising to the organic chemists—perhaps because it didn't have to any more.

⁵⁷ That is, the last within the time period 1956-1969.



Our A-60A NMR spectrometer... and its standard accessories.

Service Engineer—Does more than just install your A-60A. Makes sure it meets (or exceeds) our published specs. Trains you and your staff in all phases of operation and routine maintenance. Also provides expert service for repairs, calibration, and general maintenance.

Spare Parts and Supplies Supervisor—Sees that you get immediate delivery from our shelf stock when you need spare parts or supplies. By air in emergencies.

Marketing Engineer—Is trained to advise and recommend the combination of equipment best suited to your needs.

Research Scientist—Presides at our annual NMR workshops and lectures. Sees to it that you get the opportunity

to consult with our scientists and service engineers.

Applications Chemist—Assists you with any unusual or difficult NMR application.

If you think our A-60A and its standard accessories would be valuable to you, write for complete information to 611 Hansen Way, Palo Alto, California 94303.



varian
analytical instrument division

Figure 4. "Our A60-A NMR spectrometer and its standard accessories"

Chapter 4: Conclusion: NMR Spectrometers and *Domains of Knowledge*

In the previous pages, I have examined the growth of Nuclear Magnetic Resonance (NMR) Spectroscopy in the field of organic chemistry as seen from the vantage points of the organic chemists and Varian Associates—the makers of the first spectrometers. To understand how the organic chemists took part in this shaping, we looked at the abstracts for articles printed in the *Journal of Organic Chemistry* between the years 1956 and 1969 that referenced the use of NMR spectrometers in their experimental activities. We explored several developments in NMR spectroscopy that the organic chemists took part in creating, including the expansion of NMR studies to new substances, developing spectroscopic methods for elements other than H¹, the use of the instrument as a quantitative tool, using NMR spectroscopy for stereochemical studies, the dramatic increase in the number of samples coming under study, and the further development of new methods and specialized solvents designed specifically for use in NMR spectrometers.

To study the role of Varian Associates in the development of NMR spectroscopy as an investigative tool for organic chemists, I have examined the advertisements published by the company in the *Journal of Organic Chemistry* in the same time mentioned above and placed these ads in the context of the company's own development.⁵⁸ We have paid special attention to the ads run by Varian known as the “NMR at Work” series. Within these advertisements, Varian Associates actively engaged the field of organic chemists in intellectual conversation while at the same time attempting to create space for a new instrument in an already crowded marketplace. Understanding how the advertisements

⁵⁸ Provided by Lenoir and Lécuyer (1995).

changed over the years has helped to uncover how the instrument—physically and conceptually—has also changed.

In light of these investigations, three points arise that warrant further discussion: 1) the partnership between the organic chemists and Varian Associates, 2) the changing identity of the NMR spectrometer, and 3) the relation between the NMR spectrometer and the *domain of knowledge* known as NMR spectroscopy. While each closing thought stands alone, each also finds itself linked within the network of this story. I will take each in turn, but I will also point out connections between them.

4.1 Organic chemists, Varian, and the co-development of NMR spectroscopy

I stated earlier that the creation of NMR spectroscopy is a complex story that involves many players, with different goals, many obstacles standing in the way of those goals, and a multitude of possible paths to attain them. As I have shown, a number of players, including the organic chemists and Varian Associates, worked together to create what became known as the field of NMR spectroscopy. Both groups played integral roles as co-creators. It is for this reason that the story of NMR spectroscopy cannot be told completely from one perspective. In several instances, between the years 1956 and 1969, major developments were made possible by close cooperation between organic chemists and Varian involving the pursuit of common goals.

In the time between 1956 and 1969, these collaborative efforts transformed NMR spectrometers transformed from instruments with tremendous theoretical capabilities, but a much narrower spectrum of practical applications, to dynamic instruments capable of a multitude of operations. Varian expanded the practical analytical capabilities of the spectrometers to include elements beyond H^1 for increased ability in structural

determinations. Chemists responded by publishing a number of articles utilizing the extended analytical function of their spectrometers. Chemists working in labs that examined natural products had only chemical means of separation available when analyzing a sample that contained a mixture of compounds. Varian responded by pushing the quantitative abilities of its instrument. Chemists, also, naturally wanted the ability to analyze more samples faster. Varian responded by inserting the components like the C-1024 time-averaging computer into their instrument. They also developed instruments that required fewer calibrations, and took up smaller amounts of lab space. The chemists responded by publishing more papers that relied on NMR spectra as a means of analytical proof. As NMR became a credible tool for analysis, more chemists desired access to these instruments. In response, Varian opened two new Application Laboratories (in Pittsburgh, PA and Zug, Switzerland) so that chemists could visit and discuss the latest analytical developments and complications. As chemists became more familiar with the instrument and its actual and potential capabilities, new solvents were developed specifically for use in NMR spectrometers and new methods were developed that would maximize the amount of information that a chemist could obtain from the instrument. And so the story of NMR goes...

Within this dynamic relationship, organic chemists and Varian Associates both took part in changing the identity of the instrument with which they worked. With each new application and each new advertisement, the answer to the question, "What is an NMR spectrometer?" had the potential for change.

4.2 What is an NMR spectrometer?

Every time a chemist used an NMR spectrometer in a new way, or Varian advertised their machines as capable of some new function, an attempt was made to alter the identity of the NMR spectrometer. Thus, answering the question, “What is an NMR spectrometer?” becomes increasingly difficult outside of its historical and cultural context. The NMR spectrometer used by Norman Allinger in 1956 to investigate the structure of helvolic acid was definitely physically different from the NMR spectrometer used by Pletcher and Cordes in 1967 when they examined the basicity and coupling constants of three groups of compounds. But, the instrument did not undergo only physical changes. Within the years 1956 and 1969, attempts to transform NMR spectrometers were made time and again by the players involved in the creation of NMR spectroscopy.

What, then, do we gain by asking the question, “What is an NMR spectrometer?” That is, besides the technological changes that took place, what else does asking this question uncover? Inevitably, it is the very perceived identity of the instrument that we are looking for here. An instrument is more than a collection of technological artifacts assembled to perform a designated function—although, it is also that. There is something more to the instrument that changes when the chemist (or physicist, or biologist, or doctor, or geologist...) attempts to use it in a new or novel way. The instrument changes conceptually for the researcher—and, through the researcher’s interaction within her/his community, the perception of the instrument changes on a much broader scale. The first NMR spectrometer ever used by an organic chemist had an identity. The instrument was designed and used to answer a pre-conceived set of questions with an equally predictable set of acceptable answers. When that same instrument was used to perform a function *not* established to be *standard*—for instance the first time a chemist decided to study the

shielding affects of a particular structural conformation with the instrument—the researcher was attempting to alter the identity of the NMR spectrometer.⁵⁹ If we accept that the answer to the question, “What is an NMR spectrometer?” is necessarily tied to the question, “What is an NMR spectrometer used for?” then it becomes clear that this expansion of possible uses has the potential to change our response to the former question—and, thus, we could have a *different* instrument. Although the instrument remained technologically the same, conceptually the instrument was altered.

Changes in advertisements, too, had the potential to change the identity of the instrument. When Varian began marketing the NMR spectrometer, the company spoke of the abilities of the instrument. They were guaranteeing the chemists access to a certain set of information if they chose to use their instrument for analytical work. The details of those advertisements changed as the instrument was re-tooled and re-interpreted. As I noted above, Varian not only set temporary guidelines for organic chemists to follow, they also responded to the demands of those same chemists. Researchers and designers at Varian were inclined to work with marketers and financial officers to ensure that the chemists received what they wanted. These various members of the company, then, were forced to confront the same question that organic chemists faced, “What is an NMR spectrometer?” Without an answer to this question, there would have been no advertisements, no new model developments, and no technological artifact that we call an NMR spectrometer. The NMR spectrometer described to us in “NMR at Work” #48 is not the same Varian described in #97 eight years later. Again, the instrument had changed technologically, but it had also changed conceptually. Varian could not have imagined the spectrometer of 1966 in 1958. The instruments were simply different.

⁵⁹ Not necessarily the same *exact* instrument, but the same model with the same features as determined by Varian to be “standard.”

These identity changes cannot be marked by single events. We cannot look at one (or several) specific instance(s) and say, “There...NMR spectrometers were this, but now they are that.” No, the identity of the instrument is something that is constantly being negotiated, and the factors involved in this negotiation were simply too numerous and too complicated to allow for this type of demarcation. The identity of the instrument, after all, involved much more than the design and use of the instrument. The identity of the instrument had to be linked to theoretical understandings involved with the design and use of the instrument, experimental practice of those using the instrument, and—perhaps most importantly—the broader societal location of the instrument. This is why I must speak of “attempts” to alter the identity. While organic chemists and researchers at Varian could attempt to change what the NMR spectrometer was, they were confined by their own existence within a broader social fabric.⁶⁰ Through these means, then, the identity of the instrument was negotiated.

This negotiation, as we have seen, takes many forms. Chemists did their part by exploring new facets of the instrument. They asked new questions and expected new answers. They designed new solvents and methods of analysis. They analyzed new types of substances. They analyzed more substances, faster. They eventually saw certain types of analysis as “standard” or “fundamental,” and saw others as “cutting-edge” or “novel.” Varian, too, took part in these negotiations. They described their instruments in the pages of the *Journal of Organic Chemistry*. They assisted researchers in analyzing materials and organized forums for discussion about their new instruments. They sold chemists on specific features of the instrument at different times. They added new hardware to their old instruments and

⁶⁰ I use the image of the Go board to understand how organic chemists (or Varian) could attempt to open new areas for movement. These moves only created a space for action if others acknowledged that move (i.e., another player decided to address the move with a move of their own in at same region). The Go board image is described in greater detail below.

made new models to incorporate more new ideas of what an NMR spectrometer could be. The dialogue between these two players—the organic chemists and Varian—helped to establish the field of NMR spectroscopy and to continuously reinvent the instrument that remained central to these investigations. But, why all of this emphasis on trying to answer the question, “What is an NMR spectrometer?” What does understanding the attempts made to change the nature of the instrument show us? More than just the identity of the instrument was at stake.

4.3 The NMR spectrometer and the domain of knowledge

In the introduction, I briefly introduced the idea of the *domain of knowledge*. In order to understand how this notion fits with our case, I will describe some characteristics of domains before talking about what role the NMR spectrometer—as an instrument—played in defining and providing access to the domain of NMR spectroscopy.

I imagine a seamless network that spans equally in all directions.⁶¹ Within this network, all things human and material exist.⁶² Within this network, then, we have the organic chemists, Varian Associates, the physicists, independent chemical producers, lab technicians, magnets, chemicals, radio receivers, laboratory managers, the editors of the *Journal of Organic Chemistry*, and a host of other players that all had a role in the creation of NMR spectroscopy. Here, as I mentioned in the introduction, we have focused on only two of these players—the organic chemists and Varian. It should be evident by now that I could have focused on many others who played a crucial role in the development of NMR

⁶¹ Naturally, certain works dealing with actor-network theory have inspired this type of imagery, including Callon (1986) and Latour (1987). But I am also thinking here of Deleuze’s “plane of consistency” as developed in Deleuze and Guattari (1987)—a plane where the present takes place and all things in that immediate present exist.

⁶² This is, perhaps, an artificial distinction, but I word it this way to ensure that we understand that *all* types of agents exist within this network.

spectroscopy. It should also be clear that none of these individuals, groups, or material agents could have brought about the creation of NMR spectroscopy alone. The alliances formed between the organic chemists and Varian, for instance, were not merely partnerships of convenience, but necessary to reach the goals that each of the groups had. It is within the fabric of this network that these alliances formed.⁶³ What, then, is a *domain*, and how does it come out of this concept of the network?

The *domain* comes from the work of a certain set of actors who have chosen to work together in order to reach their goals. As they work and create knowledge, the participants work within certain constraints while at the same time working to create what those limits will be. The imagery of the Go board proves useful in explaining this.⁶⁴ In the beginning, all moves are possible, and the players are free to move however they like. But as the game progresses, their choice of movements becomes constrained—by the moves of the other players and their own previous moves. Their decisions, then, are not directed only by their will, but by the wills of the other players. If their field of vision is too narrow, they can become lost in the current area of action—an area where eventually all space will be filled—and they will run out of moves. However, periodically, a player may choose to make a move in a new area of the board. This new area may provide them with greater freedom of movement, which allows them to attempt to guide the moves of the others into a new region. This move does not free any of the players from the previously established constraints. The moves made in the past continue to play a role in how they choose to place their pieces in this new area of the board. But, by moving into a new space, a player can

⁶³ Here, I am thinking of Callon's (1987) discussion of "enrollment," which seeks to explain why certain agents work together to try and reach an agreed upon goal and sometimes requires the agents to rethink their initial goals and modify them slightly. I find this concept very helpful for thinking through the case of NMR spectroscopy. However, I do not want to adopt all of Callon's language here (for instance, his discussion of the obligatory passage point [OPP])...at least not at this time.

⁶⁴ The image of the Go board is also discussed by Deleuze and Guattari (1987) and Latour (1986) and (1987).

produce the freedom to work with the past moves in a new—perhaps less confining—way. The other players now have additional options as well. They can continue to place pieces in the abandoned territory, address the moves made in the new territory, or make a move into a new area, themselves. As the game moves forward, the players will again come to constrain themselves and one another—but they will also have the option to seek out new territory. However, unlike a Go board, this network has no “end.” There are no solid boundaries that forbid movement and eventually bring the game to a close. Additionally, new players can join the game at any time, just as current players can bow out whenever they wish. While this has dramatic effects on the game being played, it is not impossible to do. The introduction of a new player can create the potential for movement in a new area while the loss of a player may make some moves previously available temporarily unavailable.⁶⁵ The series of moves continues in this fashion with *choice* standing as the only constant.

Where, then, does the *domain* figure into this picture? The domain represents the area on the surface of the board where all current moves reside. Each time one of the participating actors moves into a previously unused area of the board, the domain expands to include that new area. If the other players choose to address that move with moves of their own, that area of the domain expands to accommodate the interest in this space.

Within the bounds of this domain, knowledge production takes place. This knowledge comes in the form of both conceptual and material knowledge. New ideas arise from the organic chemists about what an NMR spectrometer can do. Their investigations lead to a clearer model of the electronic and magnetic possibilities of organic molecules. However, organic chemists also produce new chemicals—a form of material knowledge—specifically designed to work with NMR spectrometers. Concurrently, Varian works to

⁶⁵ On the “enrollment” of a new player see footnote 61 above.

rethink the possible configurations of radio receiver and magnet to optimize detection capabilities. They develop new computer components, such as the C-1024, to increase the efficiency of the instrument. They, too, are engaged in conceptual knowledge production. Like some of the organic chemists, they search for clues about the electronic and magnetic properties of certain atoms and molecules. However, one might argue that much of the knowledge being produced within this domain seems to have broad importance for areas of study outside of NMR spectroscopy. This is true, and this is why we should speak, briefly, here about the existence of other domains.

Certainly, the domain of NMR spectroscopy is not the only domain of knowledge, and the players within the domain of NMR spectroscopy do not operate in only one domain. For this reason, we must not see the broader network that these domains exist on as simply extending in two-dimensional space. Three dimensions (at the very least) are necessary to imagine how actors can take part in multiple, simultaneous, domains of knowledge. As the above case demonstrates, organic chemists played a crucial role in the development of NMR spectroscopy, but not *all* organic chemists took part in this particular area of research. Varian's story looks a little different. The company organized around the development of new instruments for the scientific community—specifically the NMR spectrometer, which would capitalize on the pioneering work of Felix Bloch. Like the organic chemists, however, Varian found itself involved in other areas of research. In the early years of the company, Varian depended to a great extent upon the work it did for the U.S. government. The development of spectrometers remained a central goal, but one that could not be funded without other outside contract work.⁶⁶ It should be evident at this point that multiple

⁶⁶ “In the early days of the company, Varian Associates was primarily a research and engineering services company. The sale of manufactured items did not exceed the earnings from research and engineering work until 1955” (Lenoir and Lécuyer [1995] p. 303).

domains can, and *must* exist. But, how do these domains interact (or at the very least coexist) with one another? If we view the technoscientific enterprise as one consisting of multiple cultures, then the interaction between domains resembles the interaction between those cultures. When two separate cultures attempt to share information, a transaction takes place between their members. These points of contact introduce issues in addition to what I have dealt with here, and require a separate investigation. To understand how these domains interact, consideration needs to be given to issues of boundaries and culture—at the very least. However interesting, discussions of these topics must be tabled for a later time.⁶⁷

At this point, two questions remain: 1) what holds this domain together, and 2) what role does the instrument, itself, play with respect to this particular *domain of knowledge*? The instrument—in this case the NMR spectrometer—embodies the knowledge contained within the domain of NMR spectroscopy. For this reason, the instrument also provides access into this particular domain. In another way, for a new player to enter the “game” of NMR spectroscopy, the player can enter via the NMR spectrometer. For this reason, the NMR spectrometer not only *embodies* the field of NMR spectroscopy, but the spectrometer also *defines* what research can be done within that domain. However, it should be clear from the previous discussion that we cannot assume this definition of the field to be rigid. While the instrument plays the role of body and definition of the field of NMR spectroscopy, the players within the field engage themselves in the constant renegotiation of the identity of the instrument and the territory of the specific *domain of knowledge*. In this way, the domain of NMR spectroscopy finds itself in a reoccurring (re/de)territorializing process (Deleuze and Guattari 1987). This reemphasizes the discussion from above concerning the Go board. The territory of the domain changes as new players enter, old players bow out, and current

⁶⁷ For boundary issues, see Gieryn (1999). The notion of separate culture in science is developed in several places. See Galison (1997), Galison and Stump (1996), and Knorr-Cetina (1998) for examples.

players make moves that lie outside the currently defined domain. Again, these changes in use and in advertising (i.e. both the conceptual and material changes of the NMR spectrometer) are attempts to alter the identity of the instrument. When these attempts are successful, a new instrument and a new definition of the domain result.

The instrument and the domain, then, are in a constant state of “becoming” (Deleuze and Guattari 1987). So long as the players continue to play, the domain of NMR spectroscopy is always being negotiated.⁶⁸ The players within the network cooperate and compete with one another to hold their ground and to create new avenues of development. Some of these new areas become incorporated into the domain, some do not, while others lead into neighboring domains—occasionally creating connections and redefining multiple domains. All the while, the instrument changes—physically and conceptually—and the answer to the question, “What is an NMR spectrometer?” has no definite end.

4.4 Future Work

As mentioned above, the concept of what an NMR spectrometer is did not solidify at the end of 1969. The instrument continued to undergo technological transformations (e.g. the addition of Fourier Transform (FT) technologies into the radio receiver) as well as conceptual transformations. The instrument also found itself being applied to new situations. In the 1970’s, Raymond Damadian began to explore applications of nuclear magnetic resonance imaging to the human body—and, thus, created MRI (magnetic

⁶⁸ I want to note here that this negotiation takes place *inside* the domain. I believe it is here that the concept of the domain becomes distinct from other concepts such as Galison’s “trading zone” (1997, esp. ch. 9). As I understand Galison’s account of trading zones, negotiations occur at the borders between cultures. There are, no doubt, many situations that fit with Galison’s account. But, in the case of the network and domain that I am describing here, these negotiations take place *within* the domain.

resonance imaging). Further research could help to elucidate how this transformation took place.

I also mentioned above that NMR was used to investigate nucleosides. Another question that one may ask, then, is what role NMR played (if any) in the “cracking” of the genetic code? How (and why) did biologists and biochemists see NMR as an integral tool for the elucidation of genetic material?

Both of these previous examples lead to the more theoretical discussions concerning the nature of the *domain of knowledge*. Investigations into how the instrument was incorporated into new domains may create an opportunity to address questions that I was unable to address here—such as: How do domains form? How do they end? How do they interact with one another? What happens to the identity of the instrument when it comes to embody the knowledge found in more than one domain? In addition to questions concerning the nature of the domain, further work could be done on the nature of the actors within the domain. An exploration into the interactions among actors could be situated into the broader discussion occurring with the field of STS revolving the unity or disunity of science, issues related to multiculturalism (i.e. viewing the “sciences” as separate cultures), and what happens in the exchange of information between these cultures.

Finally, this case brings to light certain issues concerning the nature of the supposed science/technology divide that were not fully explored here. The thesis clearly calls into question the more traditional notion that science drives technology. Organic chemists were guided in their research by the technology made available to them. While they played a role in defining what those limits were, their choosing to use NMR spectrometers directly influenced the work done in the laboratory. This issue, in addition to the ones already mentioned, all deserve serious consideration for further development.

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**Curriculum Vitae
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