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Happy 100th Birthday to HIST!

BULLETIN FOR THE HISTORY OF CHEMISTRY

VOLUME 47.1 CONTENTS
HIST CENTENNIAL ISSUE
CARMEN J. GIUNTA & JEFFREY I. SEEMAN, EDITORS

The Cover... Chairs of HIST from its first century (pp 42 and 170)

FOREWORD

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I tried to distinguish for myself what went into the writing of a "historically-informed" play by Carl Djerassi and myself, "Oxygen" (1), and the history of the discovery of that element, as investigated by many, and retold recently by Jean-Pierre Poirier (2). So obvious—a fiction vs. truth. But… trouble was lurking at every step in my thinking. Fiction could be seen transforming into hypothesis, and the vaunted truth—an ideal good for mottos, but not standing up well to analysis.

So I retreat, and write down a piece of my interior monologue in probing the distinction between a play and a history. Why not start with a definition of good history of science, which, in the context of Antoine Lavoisier, Larry Holmes (3) and Poirier (2) gave us? What I say subsequently is obvious to the professional authors in this issue. But perhaps it doesn't hurt to repeat it. Here's my try:

> Good history of science is an authentic account of scientific events, and their causes and consequences for the people involved, and the community.

The first clause tries to escape a definition of truth (see substantive article in the *Stanford Encyclopedia of Philosophy* (4)). Even if it were as simple as "the truth is the facts" (what Joseph Priestley told the Lavoisiers at an October 1774 Paris dinner about his way of making oxygen from mercuric oxide), one is immediately faced with what Antoine or Marie-Anne Paulze Lavoisier made of that statement—how they understood it. For good reasons, this has been called the Rashomon effect, recently put to good use by Jeffrey I. Seeman (5). Making you cognizant of the multiplicity of perceptions of any action, it automatically creates an interconnected network of interpretation from seemingly simple facts/datapoints, and the human beings involved. Most certainly including the historian.

The facts are mute (I have used this phrase before). It is a human being that weaves a story around the facts, a story of connection and causation. One story crafted by the scientists as they did the work. Another by the historian.

A story is constructed, based on the facts. And slowly the difference between fiction and truth is undermined. Narrative is human, narrative is natural. Elsewhere I have written of the essential nature of storytelling in science ("Narrative" (6) and "The Tensions of Scientific Storytelling" (7), both *American Scientist* columns). And how narrative, along with other modes of reasoning that are not mathematizable, such as metaphor, is undervalued in science.

It is inevitable that the historian's story is more "rational" than that of the scientist. (Shall I call him/her "the actor", inviting a resonance with theatre? And on another level, probing what is real in theatrical performance.) The historian, after all, sees more. And after time has passed. Dangerous, and seductive—that hindsight. Yet, somehow the historian's perspective of a fixed-motive actor is unrealistic. The outlook of the actor/scientist is continually adjusted, and in no way as "rationally" as the historian may wish to see him or her. The actor moves to a state of understanding or misunderstanding, struggling all the way. With facts that are waiting to be fit in, explanations that enrich and complicate the story. If the historian can change his or her analysis, why not the actor?

I find the formulation of "causes" that often occurs in historical studies, of science or otherwise, to be troubling. Even accepting the multiplicity of causative events, there is a peculiarly mechanical aspect that invoking causation attaches to human-driven events. It is somehow as if the actors, be they Lavoisier or the school-teacher who hid five of us for fifteen months in 1943-4 Ukraine (8), were automata, devoid of free will. I would prefer to see a platter laid out, with multiple small causative events displayed on it.

Also, I don't want the actor/scientist's way to be seen as quiet, rational progress—it's a scramble, a seizing of every foot- or hand-hold on understanding. I've called it scrabbling, and I do not have the board game in mind. I've found the process useful in characterizing my actions, or the actions of another scientist, prior to the sanitizing process of getting their work past the gatekeepers of scientific publication.

Am I confirming Paul Feyerabend's outlook (9) that anything goes? There may be moments of it, but somehow I feel that for most people the scrabbling is in the service of a good, that of the enhancement of reliable knowledge. We generally have no problem telling apart the intent charlatan/faker and the struggling scientist.

So let me try for another formulation:

> Good history of science is writing a detailed story of scientific work, one that makes sense.

This is going to get me into as much trouble as the first definition, if not more. "Story" is pretty vague, and there is zero incentive, it would seem to some, that the words spoken, or measurements made, are reliably reported and, where that matters, are reproducible within a margin of error.

I would counter that falsified facts and unreproducible work do not "make sense." But the Trump years and legacy would make anyone question that position.

I still believe that getting the word "story" in the description is a plus. It hints at a multiplicity of potentially credible stories, and the natural variability in their reception. It makes you think of both the actor/scientist and the historian of science engaged in the creation of a story. Making sense is a strong constraint on what both do.

Another interesting outcome of this definition is that it provides an opening to imaginative work, be it fiction or theatre. The construction of alternative realities (making good sense, of course) could then be seen as not just the province of science fiction or fantasy, or authors of fiction in general. But it could also be seen as productive activity for historians of science. Or their students!

References and Notes

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9. P. Feyerabend, *Against Method: Outline of an Anarchistic Theory of Knowledge,* Redwood Burn Ltd/Trowbridge & Esher, London, 1975.

About the Author

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PREFACE: HAPPY CENTENNIAL TO THE ACS DIVISION OF THE HISTORY OF CHEMISTRY

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> The nature of [scientific] communities provides a virtual guarantee that both the list of problems solved by science and the precision of individual problem-solutions will grow and grow. At least, the nature of the community provides such a guarantee if there is any way at all in which it can be provided. What better criterion than the decision of the scientific group could there be?
>
> —Thomas S. Kuhn, 1970 (1)

We, the co-editors of this commemorative issue of the *Bulletin for the History of Chemistry*, believe that Kuhn's words speak for the history of science as well as they do for science itself. We are more than delighted to welcome you, our readers, to this special issue of the *Bulletin*.

Indeed, we are overwhelmed by and appreciative of the responses of 16 of our colleagues to publish their articles in this special issue. These historians of chemistry and chemist-historians individually, and thus collectively, have shared their diverse ideas and visions for the future of the study of the history of chemistry. We sincerely thank them for their participation. They have joined together with a wonderful diversity of personal and professional experiences to share their mindful deep thinking and personal commitments to chemistry and to the history of chemistry. We have been stimulated by the insights and examples given in this set of essays, and we look forward to seeing future work in the history of chemistry along the lines outlined here. We are grateful as well to those who supported the project with insights and assistance behind the scenes.

These papers reveal the authors' idiosyncratic responses to the prompt we provided:

> The working theme for this special issue is: "Novel Insights in the History of Chemistry: Looking Back Yet Mostly Looking Forward." Possible subjects include:

- questions or topics ripe for exploration
- promising methodologies
- developing new audiences
- interdisciplinary opportunities
- new ways of analyzing previously studied topics

This theme led to a wide variety of responses, which we have collected together into the following six topics arranged after Roald Hoffmann's thoughtful foreword and this preface:

Expansive Approaches to the History of Chemistry

"Epitomizing Chemistry for Changing Audiences in Britain, 1820 -2020," by Robert G. W. Anderson

"Mendeleev's 'Problems:' A Means to Engage Students and Teachers in the History of Chemistry," by Arthur Greenberg

"Archaeological Chemistry: Past, Present, Future," by Mary Virginia Orna

"Can We Bring Chemistry Back? Exploring the Potential of 'Gateway Artifacts' at the Science History Institute," by David Allen Cole

Foci on Specific Topics

"Historiography of the Chemical Industry: Technologies and Products versus Corporate History," by Anthony S. Travis

"A Future History of Selectivity in Organic Chemistry: Whence, Where, and Whither?" by David E. Lewis

"The Development of Medicinal Chemistry as a Disciplines: A Topic Ripe for Historical Exploration," by John Parascandola

Multidisciplinary Approaches and Tools

"Moving Beyond the Intersection of Chemistry and History: Evolving Multidisciplinary Approaches to the Historical Study of Chemistry," by Seth C. Rasmussen

"Computational History of Chemistry," by Guillermo Restrepo

Thriving, Inclusivity, Diversity, and Equity and the History of Chemistry

"History of Chemistry as a Tool for the Engagement of Underrepresented Students in Chemistry," by Sibrina N. Collins

"Out of Obscurity: Contextualizing Forgotten Women Chemists," by Marelene F. Rayner-Canham and Geoffrey W. Rayner-Canham

Relationships of Historians and Chemist-Historians

"'The Poor Sister:' Coming to Grips with Recent and Contemporary Chemistry," by Stephen J. Weininger

The Importance of Plurality and Mutual Respect in the Practice of the History of Chemistry," by Peter J. T. Morris and Jeffrey I. Seeman

"The Long and Short of It: The Future Writing of History of Chemistry," by William H. Brock

The Past, Present and Future of History of Chemistry

"Does History of Chemistry Have a Future?" by William B. Jensen

"Remote Interviewing and the History of Chemistry," by Jeffrey I. Seeman

"Is There Room for the Present in the History of Chemistry?" by Carmen J. Giunta

"Reflections on the Last and the Next Hundred Years," by Alan J. Rocke

We happily celebrate the 100th birthday of the Division of History of Chemistry of the American Chemical Society. Happy Birthday HIST!

We encourage you, our readers, to contribute to the future of HIST. We especially invite you to submit articles to the Division's journal, the *Bulletin for the History of Chemistry*. All articles in the *Bulletin* become open access after three years; of course, they are immediately available to members of HIST. So, there are decades of papers dealing with the history of chemistry—which have a long shelf life!—available for all to read, free of charge.

We also thank the Executive Committee of HIST for providing the funds for this special issue of the *Bulletin*—two other issues will appear in 2022 as usual. Three issues of the *Bulletin* will appear in 2022, a record! Furthermore, the Executive Committee agreed with our request that this special issue be Open Access immediately.

In addition to the *Bulletin*, HIST sponsors many activities, including symposia and awards, about which more information can be found at the Division's website: acshist.scs.illinois.edu. The Division's present and future will depend on the ideas and energy of the history of chemistry community: please join us in making that future!

We dedicate this special issue to the founders of the Division of History of Chemistry of the American Chemical Society, Charles A. Browne and Edgar Fahs Smith, and to all those others who have participated in any of the activities of HIST during its first 100 years. Look for centennial features in the other 2022 issues of the *Bulletin* as well, commemorating some of those important contributors.

Reference

1. T. S. Kuhn, *The Structure of Scientific Revolutions*, 2nd ed., University of Chicago Press, Chicago, IL, 1970.

EPITOMIZING CHEMISTRY FOR CHANGING AUDIENCES IN BRITAIN, 1820-2020

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Abstract

Chemical texts which are most studied by historians of chemistry are those written by those whose work has made the most impact on shaping the discipline. Books of this kind exist to inform fellow-minded chemists, those who aspire to the same intellectual level of understanding as the authors they study. However, there is a genre of published material which is intended for those curious about the subject and yet do not aspire to become professionals themselves. Their interest in the subject is serious, not simply recreational. Over the past two centuries, when chemistry was sought-after by new audiences, changing forms of literature have been written with them in mind. A fairly well-defined group of students were those who subscribed to night classes in mechanics' institutes. They were from the poorer reaches of society and could not afford expensively produced volumes. A chance discovery has been made of a broadsheet produced by a Glasgow teacher which considers a wide sweep of the subject as it was known in the 1830s. This kind of evidence has built-in ephemerality and it is likely that other printed material of this type once existed. Later books, for a growing middle-class audience, range from a rigorous but simplified description of the science, to a discursive account of the social effects of chemistry. In the cases considered, the chemistry volumes come from a pedagogic series across a wide range of subjects. In the final text considered, one from the Very Short Introduction series, the author offers sympathy to the student because of the popular poor reputation of the subject! Necessarily, the examples chosen are highly selective. They are of a fairly balanced chronological span and hopefully can be considered as being reasonably representative. Finally, there are speculations about what the effect on the subject of the introduction of largely electronic forms of communication will be and hence on the writing of the history of chemistry in the future.

Introduction

A good deal has been published on the important subject of popularization of science in the nineteenth and twentieth centuries (1). These monographs take a broad view of the provision of scientific knowledge. This short paper looks specifically at a small selection of modest, low-priced printed works published in Great Britain (though some with co-editions in the United States) which were intended for students who in the earlier period wanted to understand chemistry through its scientific detail. Some later audiences were attracted by chemistry's role and influence on society in the books written for them.

Until the mid-eighteenth century, teaching texts covering the full breadth of chemistry, as then known, were largely published with scholars, practicing chemists, pharmacists or students attending institutional courses, and libraries, in mind. Examples are works by teachers such as Nicolas de Lemery (1646-1715), *Le Cours de Chymie*, first edition 1687; or of Herman Boerhaave (1668-1738), *Elementa Chemiae*, first edition 1732.

These were fat, expensive, textbooks, with woodcuts or engravings and often bound by the purchaser in luxurious leather bindings with gold tooling. They were soon translated into other languages. The audience for chemical knowledge had expanded through the second half of the eighteenth century and it became a fashionable social pursuit in some centers, especially Paris (2) and London (3). Contemporary printed images show both men and women of the genteel classes enjoying spectacular demonstrations being performed by their chemistry lecturers. This very occasionally led to individual long-term obsessions but by and large the courses offered were ends in themselves and publication for these wider audiences was not usual. At the beginning of the nineteenth century a few textbooks were written for other types of audience, for instance for young persons who were just starting chemical studies. One of these was Samuel Parkes' *A Chemical Catechism for the Use of Young People* of 1806, written for the education of his daughter. There were 14 editions published in England (the title was simplified to *The Chemical Catechism* for the second edition of 1807); two of them were edited by others after Parkes had died. There were also American editions. Parkes claimed that in his approach "the catechetical form, which was first chosen for this work, has been found to possess at least all the advantages that any other mode of instructing youth in chemistry can claim" (fourth edition of 1817, page vii). In the same year Jane Marcet's *Conversations on Chemistry, Intended More Especially for the Female Sex,* was first published. Its similar, though simpler catechistic style, more conversational in nature, was intended for a respectable middle-class readership, the three textual personages being a mentor ("Mrs. Bryant") who taught two young women ("Emily" and "Caroline"). The book proved to be extremely popular, passing through 16 editions published in England, and 23 American ones (4), the later ones pirated and published under the authorship of John Lee Comstock (from 1822) and Thomas P Jones (from 1831, the latter with a slight change in the title).

At the beginning of the nineteenth century science teaching became more accessible to those with limited means. In Great Britain organizations recognized this new market. In particular, the Society for the Diffusion of Useful Knowledge, was founded in 1826 largely at the instigation of Lord (Henry) Brougham and acted to encourage the spread of knowledge by making books much cheaper to produce. This arose largely from changes in printing technology and long print-runs. For these less well-off parts of the community, special colleges, or mechanics institutes were established independently from the 1820s for subscribers who had very little money to spare, but whose limited resources were compensated for by a great deal of enthusiasm to learn about scientific, and allied, subjects. All such institutes had libraries, most with lending facilities. Few books or papers today have attempted to survey the widespread printed material available, though the American chemist and historian, Edgar Fahs Smith in his *Old Chemistries* of 1927, considered books published from 1545 to 1837 (5). This brings me to the start of the period where the main focus lies, 1830 to 2012.

The stimulus for this was the discovery of a scarcely-known (perhaps even unknown) publication of the 1830s produced for poor students studying chemistry at a mechanics' institute in Glasgow. Its distinctiveness is that it presented an overview of all chemistry known at the time, printed on the single side of a broadsheet. This minimized the cost of paper and eliminated the cost of binding. It led to more general thoughts about modestly priced publications aimed at those who were less well-off but who were curious about the subject of chemistry, and at the same time lacked the background to be able to study the subject systematically and in detail. Rather little attention has been paid by historians of chemistry on textbooks of a relatively simple form, of which this is an extreme example. I shall briefly survey these from the date of my nineteenth century broadsheet, through basic chemistry texts, up to the present day, my final example being the 2012 book in the *A Very Short Introduction* series published by Oxford University Press. In the limited space I have available I shall not be able to review two other sources of serious scientific information which includes chemistry, periodicals such as *Mechanics Magazine* (from 1823), *Scientific American* (from 1845) and much more recently, *New Scientist* (from 1946), together with the current surfeit of books published to assist students to pass public examinations in chemistry.

William Grier

That many developments in chemistry education occurred in Scotland is not surprising. Education there was more readily available to those of non-established religious beliefs and practices. Moreover, medical education flourished, and it was necessary to take a course in chemistry before the M.D. could be granted. Oxford and Cambridge would not award degrees to those who did not subscribe to the Anglican persuasion (the 39 Articles of Religion), while the ancient universities in Scotland, St. Andrew's, Aberdeen, Glasgow and Edinburgh, offered no impediment to those whose religious beliefs differed from those of the established Church of England. As a subject connected to medicine, chemistry flourished in comparison with the languid situation south of the Border (6). As well as rigorous teaching taking place, at least in Edinburgh and Glasgow, there was a flourishing contingent of private lecturers teaching chemistry extramurally, and if these teachers were qualified, their courses could count towards fulfilling degree requirements.

In addition to the four ancient universities in Scotland, a new institution of higher education, largely to teach scientific and technical subjects part-time, was established in 1796 with a legacy from a former professor of natural philosophy at Glasgow University, John Anderson (1726-1796). The Andersonian Institution existed to teach those of modest means who had not had the benefit of traditional education, and it is very likely that the author of the broadsheet under discussion, William Grier, attended its classes. Amongst the early teachers at the Andersonian was George Birkbeck who, more than anyone else, was responsible for establishing mechanics institutions from the 1820s.

William Grier was clearly active as a teacher in Glasgow. It is known that he taught mechanics and chemistry at the Gorbals Popular Institution for the Diffusion of Science in the session 1838-39 (7). His sole contribution to chemistry publication was the Chart and he was publicly better known as being the author of books on engineering and arithmetic which went through multiple editions in Great Britain and the United States. These are *The Mechanic's Calculator* (first edition Glasgow, 1832, 18th edition Glasgow, 1856, American editions all from the Glasgow 5th edition of 1838: Philadelphia 1839, New York 1853, Hartford, 1867); *The Mechanic's Pocket Dictionary* (second edition 1837, 14th edition 1861); *The Modern Mechanic* Boston 1857 and 1861. The *Mechanic's Calculator* and *The Modern Mechanic* appear to be the same work but with the Boston editions retitled. Like the *Chart of the Science of Chemistry*, nearly all the Glasgow editions of Grier's books on engineering were published by W G Blackie & Son of Queen Street, Glasgow. The exception is the very first edition of *The Mechanic's Calculator* of 1832, published by Andrew Lottimor and James Lumsden of Glasgow. This may imply that the *Chart* was published post-1832 but by 1835.

Grier's *Chart* is a curious survival. The copy found at a London book fair in the 1990s may be the only one still to exist. Ephemeral material of this nature is not generally beloved by librarians and even specialist libraries may have decided to disregard this form of publication over the years. Mechanics' Institutes issued significant quantities of pamphlets—this is proved by the annual reports which they issued but it is not unusual for only a single, or a few of them to be preserved. It is quite possible that Grier's publication was one of several of the type which lecturers handed to their students. Nevertheless they can be valuable to historians. As an example, the (now rare) first annual report of the Edinburgh School of Arts (8) lists the occupations of its first tranche of 25 students as being cabinet-makers, gardeners, a weaver, an iron-founder, and a fishing-rod maker—and several others. The report provides much further information about its first year of operation, including the syllabus of Andrew Fyfe's chemistry course, the catalogue of the library, the accounts, and a long list of the many subscribers.

Compared with a good number of other contemporary teachers in Scottish mechanics' institutes, William Grier is a little-known figure, and his dates of birth and death still remain to be discovered. What little is now known of Grier comes largely from the substantial introductions he wrote for his published works and in them he makes some interesting points, though perhaps they are not unexpected from one who started off from a modest background. He presages the philosophy of Samuel Smiles's *Self-Help* of some twenty years later, in a passage

> The man who would relinquish scientific pursuits because he had no hope of reaching the eminence of a Newton, a Watt, or a Davy is no better than him, who, in despair of ever obtaining a share of wealth equal to that of the rich inheritor of the land, would cease to make any honest exertion to raise himself from a state of the most squalid wretchedness. [*Calculator*, p 5]

There is an indication that he may have attended classes at Anderson's Institution:

> In the museum of the mechanic's class founded by the venerable Anderson of Glasgow, there is preserved the model of a machine to procure a perpetual motion … But had [its maker] been acquainted with the first principles of mechanics … he would have seen the utter folly of his enterprise. [p 10]

Grier declares the reason for his publication:

> This book has been written with the view of assisting the young workman in obtaining a knowledge of the calculations connected with machinery. [p 11]

Grier praises the Society for the Diffusion of Useful Knowledge: "The treatises published [by the SDUK] cannot be too warmly recommended; and are easy of access from their cheapness and mode of publication." He suggests that self-education is a duty:

> The diffusion of scientific knowledge among the working classes becomes thus not only a duty which every man owes to his country, but, besides this, it is an act of benevolence, as it tends to administer pleasure to a class of most useful men, who, in a multitude of cases, suffer grievous privations. [p 16]

The title pages of his books describe him as he wished to be known: his recurring appellation is “Civil Engineer.” But in the 3rd edition of *The Mechanic’s Pocket Dictionary* of 1838 he additionally refers to himself as “Lecturer on Natural Philosophy, Author of ‘The Mechanic’s Calculator,’ ‘A Chart of the Science of Chemistry,’ &c, &c.”

A CHART OF THE SCIENCE OF CHEMISTRY,
EMBRACING A VIEW OF THE LAWS OF CHEMICAL ACTION, AND OF THE COMPOSITION AND PROPERTIES OF INORGANIC AND ORGANIC SUBSTANCES.
BY WILLIAM GRIER,
AUTHOR OF THE MECHANIC'S CALCULATOR, &c. &c.

Figure 1. *Grier’s broadsheet, “Chart of the Science of Chemistry,” illustrating how densely packed with information is the 24 × 18 inch (61 × 47 cm) sheet.*

A Chart of the Science of Chemistry

The title of the broadsheet is: A CHART OF THE SCIENCE OF CHEMISTRY, / EMBRACING A VIEW OF THE LAWS OF CHEMICAL ACTION, AND OF THE COMPOSITION AND PROPERTIES OF INORGANIC AND ORGANIC SUBSTANCES / BY WILLIAM GRIER, / AUTHOR OF THE MECHANIC’S CALCULATOR, &c., &c.

At the bottom of the chart are production details: it was published by Blackie & Son of Queen Street, Glasgow (who published practically all of Grier’s output) and it was printed by W. G. Blackie & Co. It is undated. Another similar teaching publication, originating in Glasgow and printed on a single side of paper, dealt with the Linnaean System of botany (9).

The Grier broadsheet is printed on one side only, the printed area being 24 × 18 inches (approx. 61 × 47 cm). The size of the type is very small, probably 6 point and it is difficult to read without a magnifying glass (a limitation, one might think, for middle-aged Glasgow workmen). The chart is divided into seven vertical columns (not all of the same width). The first five are labelled “General Principles” and the last two “Organic Substances.” The rows themselves are headed (1) Chemistry, Chemical Properties, Chemical Nomenclature, Of the Properties in which Bodies Unite and Chemical Conservation, Affinity, Of the Atomic Theory and Theory of Volumes. (2) Caloric, Light, Electricity, Magnetism. (3) Simple Substances. (4) [A very long list of chemical substances in alphabetical order, from Acetic Acid to Zirconium, Sulphate of; the next three sub-columns give compositional details]. (5) Properties and Preparations. (6) Organic Substances, &c. (7) Organic Preparations. Row 7 also includes four line-engravings showing Crucibles, Distillation apparatus using a retort, Demonstration gasometer, and Woulfe’s Apparatus.

The question is, who were Grier’s influences when he was putting his broadsheet together? The most likely candidate would seem to be Andrew Ure (1778-1857), who taught chemistry at the Andersonian from 1804 to 1830. However, Ure did not publish a chemistry textbook of the kind which would allow comparisons to be made.

Precursors

Two chemistry books in rather different styles, whose texts were clearly intended for workers rather than middle-class young ladies, were provided by Andrew Fyfe (1792-1861) and John Joseph Griffin (1802-1877). Both had strong ties to the mechanics’ institute movement in Scotland though their careers followed different trajectories. Fyfe graduated in medicine from the University of Edinburgh, later also becoming a fellow (later President) of the Royal College of Surgeons. He started his career by teaching as a private lecturer in Edinburgh (10), and tried for several academic jobs. It took him 30 years before he was able to secure a post as Professor of Chemistry in Aberdeen. An early publication of his makes reference to his extra-mural teaching, *Elements of Chemistry ... Comprising the Principal Part of a Manual of Chemistry for the Use of Pupils of Mechanics Institutions* (Richardson and Lord: Boston, 1827).

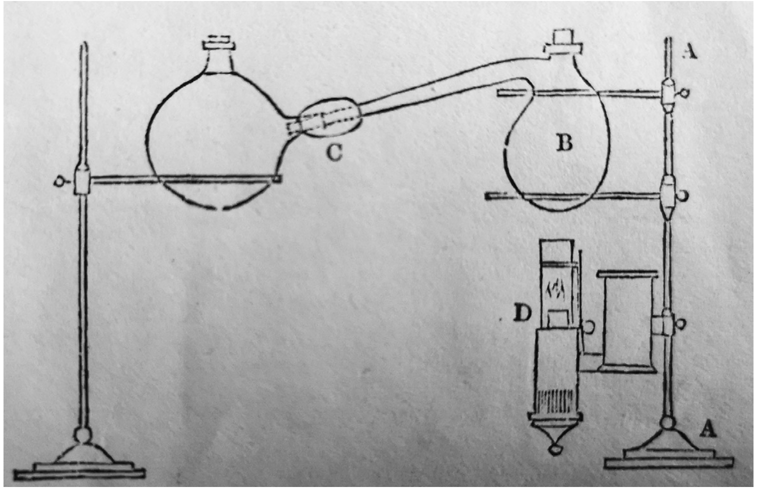

Figure 2. *Detail from Grier's broadsheet depicting a "distillatory apparatus."*

John Joseph Griffin's audience for chemistry may have had similarities yet his chemistry focus was fundamentally different (11). He, too, started his chemistry study at the Andersonian Institution, later teaching in its mechanics class. But then he became involved in the supply of chemical apparatus and in publishing, in 1823, the first of six editions of *Chemical Recreations.* In 1829 he travelled to Heidelberg in Germany to improve his knowledge of chemistry. Returning to Glasgow he continued to publish texts which closely connected with his increasingly burgeoning apparatus and instrument business. The second edition of *Chemical Recreations* of 1825 is composed of two parts, "First Lines of Chemistry," and then, "On Chemical Operations and Processes." The former starts by asking the questions which a student at Griffin's mechanics' class might well ask: "What is Chemistry?—Is it interesting?—Is it useful?—How am I to proceed in studying it?" The answer Griffin wants to hear is of course, yes. A couple of pages further on is a section Make Experiments, and here Griffin writes,

> It has been found that all the marvelous diversity of appearance under which bodies are presented to the eye, and the changes of state to which they are incessantly subjected are occasioned by the reciprocal actions and combinations of a few unchangeable primary bodies. The properties of these bodies, and the nature of the laws which regulate these actions, are therefore the object of which the chemical student is to enter into an investigation.

Griffin's company could supply the necessary simple apparatus. Some copies of *Chemical Recreations* (for example the tenth edition of 1854) have bound in the back of them copies of *Griffin's Scientific Circular* of December 1850, a catalogue advertising its wares. These included complete sets of chemical apparatus in various forms enabling students to repeat some or all of the experiments described in the front part of the book. The question has to be asked, was all the apparatus listed in the extensive catalogue immediately available, did it have to be ordered, and who in fact constructed it if it were not Griffin's own firm?

Successors

A later Scottish initiative for helping students from modest backgrounds to study and understand chemistry was that developed by a medical graduate who had a taste for chemistry rather than medicine, George Wilson (1818-1859) (12). He taught at the Edinburgh School of Arts (a very early, perhaps the first, mechanics' institute, founded 1821). In 1854 he was appointed director of the newly established Industrial Museum of Scotland whose origins lay in the Great Exhibition of 1851. His predilection was to teach industrial chemistry and he set about garnering materials for his museum from friendly local industrialists, even though an exhibition building did not yet exist (he had to store his burgeoning collection in a warehouse and a disused chapel (13)). He did teach, however, and he toured his students round local industrial works. His 1850 pedagogic textbook, *Chemistry*, whose opening paragraph declares,

> It would be of great advantage to the beginner in Chemistry if it were possible to give a simple but sufficient definition of the nature of the science on the study of which he is about to enter…

was published in the Chambers Educational Course series, and is more traditional in structure than Wilson's innovative teaching methods might have indicated. It appeared in only one edition, perhaps because he died in 1859, at a relatively young age and he had no successor as editor.

Another, rather different way of teaching, though also by using material objects, was developed by Thomas Twining (1806-1895), a wealthy merchant of the tea-importing family, who was obsessed with teaching applied science to socially and financially disadvantaged students. He did this through the medium of his Economic Museum at Twickenham, situated just outside London. He wrote in the heavily pedagogic text, intended for teachers who were expected to follow his instructive text (14),

> …this Course, besides supplying to the Working Classes in an easy and familiar style the Elementary

> and Applied Science they constantly require for their guidance in Daily Life, is intended to afford the Artisan Students a stepping-stone to further Scientific and Technical Studies…

In his teachers' text, Twining recommends chemical apparatus and glassware which were available from J. J. Griffin and Sons, and other firms.

Post-Mechanics Institutes and New Publications

Mechanics' institutes could be said to have been a great success over the first twenty or thirty years of their existence, when it has been estimated that between 400,000 and 600,000 attended some course or other in the period from 1820 to the middle of the nineteenth century. But for a number of reasons they were not sustainable. Their existence was financially precarious and philanthropy could divert their purpose, with gentrification becoming a threat to the purity of their initial aims. More access to public education by the state establishing elementary schools meant that learning moved towards different institutions. The large initial numbers may have been due to the slack being taken up from previous unavailability of courses. The nature of the earlier body of mechanics and artisans was changing. Working Men's Colleges, backed by the Christian Socialist movement, were set up from 1854 (with F D Maurice and John Ruskin heavily involved). Half a century later in 1903, An Association to Promote the Higher Education of Working Men, shortly afterwards renamed the Workers Educational Association, became an informal middle-class movement of evening classes (it still exists today). Then in 1969 the Open University was founded which has developed a vast quantity of chemistry teaching material (which it is impossible to survey here). With these changes, the nature of associated literature also changed. In this final section I shall consider three series of books which covered a very wide range of topics (chemistry amongst them) and which were printed in very large numbers. These are Benn's Sixpenny Library, the Teach Yourself Books and the Very Short Introduction series developed by Oxford University Press.

Benn's Sixpenny Library, through its very title, emphasized the cheapness of its literature. The series was produced by Ernest Benn Limited, with most of the volume titles, about one hundred of them, appearing between 1927 and 1930 at a rate of one per fortnight. *Chemistry* was published in 1927 and is numbered 104 (though it was one of the first twelve titles). The author was Percy F. Spielmann, who immediately declared pessimistically in his Foreword,

> The presentation of a comprehensive survey of a vast subject, compressed into a very limited space, and addressed to a public that is, in a great measure, unfamiliar with scientific matters, is a task of some difficulty.

Spielmann's survey occupies a mere 80 pages. However, the book is not so much about the science of chemistry, rather than about the place of chemistry in society. For example, Chapter 5 (of 7) bears the title "The Application of Chemistry to Human Affairs." In this chapter, Spielmann sees his subject as an élite calling, writing,

> It should be needless to state that the development of science as a whole and chemistry in particular is so difficult and arduous that only the fully trained are fit to attempt it…

And later,

> at the moment of writing, the demand for the services of chemists is such as to require that boys shall take up chemistry only if their bent is so strong that they cannot be kept away from it … It is very undesirable for an ill-educated individual to take chemistry.

If this is a strange thing to write in a book which might be expected to encourage readers to become interested in the subject, it is difficult to understand why Benn's Library chose Spielmann as their author. True, he was possessor of a Ph.D. and an Associate of the Royal Institute of Chemistry. His publications reveal his main interest as being bitumen and asphalt (15). A consuming interest was collecting miniature books and he published a catalogue of them (16). In his Benn's Sixpenny Library, Spielmann's approach fulfilled less of a particular need for the facts of chemistry rather more about how chemistry fitted into society.

This is in contrast to the *Teach Yourself Books* approach, which attempted to epitomize the major aspects of chemical knowledge of the day. The *Teach Yourself Books: Chemistry*. A *Practical Book of Self-Instruction in Chemistry, Based on the Work by James Knight, M.A., B.Sc., Completely Revised and Enlarged by G. Bruce MacAlpine, B.Sc.* is derived from *The Self-Educator in Chemistry* of 1901 written by James Knight (1860-1936), a Glasgow schoolmaster (though one who in fact had been awarded a D.Sc). The rationale for writing the work is clarified in the Introduction, where the author is critical of the lack of science teaching in schools, writing (17),

> This book is intended for all who wish to keep abreast of their daily reading and daily tasks. and who, by

> reason of a one-sided system of culture in youth, have felt themselves in matters relating to the outside world as the stranger within or even outside the gates.

The book filled a gap, according to a review in Durham University's *The Northerner*, which made the point, "Books on chemistry for the general reader are almost non-existent" (18). In the 1962 edition, within 240 pages, there are nineteen short chapters, two of which could be considered biochemistry (Food and Vitamins) and one on Photography. The first chapter dives right in, treating the atomic theory, followed by chemical nomenclature. From then on, most chapters are based on the chemistry of particular elements. The text is discursive; mathematics and chemical equations are used sparingly. The final chapter deals with the elements as set out in the periodic table. The overall feel of this Teach Yourself book was worthy, but presentationally dull, the dullness not being overcome by the unsubtle, garish yellow and black cover. In recent years the *Teach Yourself* series has had a rebirth (19) and is now published in a somewhat different form and with new titles, deriving from the original concept, by the publisher Random House.

As a final example of texts developed for the non-specialist, curious amateur there is the *A Very Short Introduction* (VSI) series. Here, the card covers are colored with bands of color, each one different for each title. The program of developing a multi-volume series was devised by Oxford University Press in 1995. Its success has been phenomenal—by the end of 2021 there will be about 680 volumes in the series, and in the long-term, it is expected that there will be 1,250 titles. Currently about 8 million copies have been sold. Translations have appeared in 45 languages. Most books in the series contain about 100 pages, though some are significantly longer (*Organic Chemistry*, by Graham Patrick, is 175 pages long.) It should be noted that there is a *History of Chemistry* volume in this series by William H. Brock, published in 2016 (20). The *Very Short Introduction* volumes are today's intellectual *livres de poche* for a long air-flight. The chemistry volumes need to be seen in the context of the VSI project, and its public reception, as a whole.

The author of *Chemistry: A Very Short Introduction* (numbered 417), which appeared in February 2015, is Peter Atkins, professor emeritus at the University of Oxford, who has done much to popularize his subject. There are several other *Very Short* volumes which concern chemistry, and *Physical Chemistry*, also written by Atkins, was published earlier, in 2014. Atkins starts off in a jauntily pessimistic style:

> I hope to open your eyes and show you a fascinating, Intellectually and economically, world, that of chemistry. Chemistry, I have to admit, has an unhappy reputation. People remember it from their schooldays as a subject that was largely incomprehensible, fact-rich but understanding-poor, smelly and so far removed from the real world of events and pleasures that there seemed little point in coming to terms with its grubby concepts, spells, recipes and rules.

The jaunty style continues through the book, making the text attractive and non-threatening for the layman (though there are a few fairly tough passages). There are no chemical equations to intimidate (and no diagrams), not even in the "Its [Chemistry's] Reactions" chapter. Much of the text is not so much an epitome of the science of chemistry but more of an explanation of its culture. Where does this lead the reader who yearns for more? In the Further Reading section, the first four (of seven) books recommended are works of Atkins himself—on Thermodynamics, Physical Chemistry, Atoms and Chemical Principles. This is not unfair as he is aware of writing in a sympathetic style for his uninitiated readership. Writing about the power of quantum mechanics, Atkins admits,

> that it remains largely incomprehensible is admittedly an irksome deficiency, but in due course I shall do my best to distil from it what is necessary for understanding the behaviour of atoms… [p 4]

He is being realistic; not all authors of popularizing texts are.

Approach and Conclusions

The production of texts to make chemistry, which has always been a complicated, complex subject, comprehensible to a willing but not scientifically sophisticated audience goes back well over two hundred years. In London, Edinburgh and Paris chemistry courses for an enthusiastic public (including women) were a fashionable, serious diversion for the middle classes. The audience for its study developed significantly with an upwardly shifting demographic and access to basic education of working men and women, and this provided potential for authors to develop new ways of providing for the changing readership. Early teachers at mechanics' institutes struggled to teach in a non-mathematical way, but the breadth of the scientific agenda was not compromised. This is demonstrated by Grier's broadsheet. However, authors appreciated that the developing science had to be pruned for non-specialists, and ultimately in their popularizing publications, the notion of what chemistry was became more socially based. This occurred particularly in the twentieth century and now today, Peter Atkins in his *Very Short Introduction,* has been realistic about what has been possible, and though he only hints at it, what is better left out.

What can be learned from the texts which have been used to compile this paper? It is clear that even in the earliest production, Grier's broadsheet, the content had to be highly selective in what it incorporated, even if the impression Grier may have wished to suggest to his mechanics' class was comprehensiveness. One only has to consult the earliest chemical journal, August Crell's *Chemisches Journal*, an abstracting publication, to realize that the subject had spread its wings widely even by the late eighteenth century. Crell was responsible for a total of 31 volumes over 20 years (the titles changed several times between 1778 and 1791) (21). So those who were teaching and popularizing the subject, even at this early stage, had to be highly selective in what they could teach and write. For later periods, one only has to be confronted by groaning shelves of 8000 volumes of *Chemical Abstracts* (1909 to the present) to be totally intimidated by the impossibility of the task. An important issue arising from this comparison is the level of understandability which might be expected even from the highly curious, but non-specialist seeker after knowledge. The sheer quantity of specialized chemical knowledge today is staggering and even highly competent professionals in one field are unlikely to have a grasp in areas outside their areas of expertise.

Creators of epitomizing texts have to think a great deal about how they approach the process of selectivity. It could be argued that the tendency has always been to over-consider "classic" publications and papers. The backgrounds to these inevitably have been developed by their own authors' selective readings. There is bound to be distortion about what the subject of chemistry comprises. The significance of published papers can certainly change with time. Some works now seen as seminal were ignored until many years after they had been first authored. On the other hand, some chemists of the past have become today's heroic figures and may be over-represented by compilers in how much attention they pay to them. It could be argued that the Nobel Prize holds a responsibility for some of this distortion.

The few examples I have chosen to consult and write about can only be representational of a considerable publishing phenomenon. An effort has been made to balance the chronology of these popularizing texts from the early nineteenth to the early twenty-first century, the books chosen being published in English in Great Britain, with co-editions later appearing in the United States.

The Future

Where to next? Chemistry has become a hot potato for many members of society, with its strong social and political connotations. A major current example is global warming caused by fossil fuel emissions which are the concerns of many individuals, while governments struggle with the problem which has economic as well as scientific and social consequences and which cannot be ignored (22). Teaching chemistry through publications in earlier days, by ploughing through the properties of elements one by one, is no longer a viable approach. And yet writing about chemistry while leaving out its science is fatuous and does not lead to an understanding which underlies the issues. Some compromise between the approaches is needed. To understand today's chemistry, as well as the part it plays in daily life, a willingness is needed to confront concepts which for most are unfamiliar. But this has always been the case ever since chemistry entered the domain of the curious and studious amateur two centuries ago. It seems unlikely that the reading public will ever be able to keep up with the changes in concepts and content in the future. Chemists may be able to make sense of each others' work, but even the most curious of the curious public will lag further and further behind. Chemistry historians are confronted with this problem now and will face the problem increasingly in the future. Practically no papers in history of science journals deal with near-contemporary subjects, for several reasons. Those with training in history are unlikely to have knowledge of modern or contemporary science, while scientists who take an interest in history may find it difficult to satisfy historians (who control history of science journals) (23). It is interesting that some nations have societies both for chemistry historians and also for chemists with strong historical interests. In Great Britain, the Society for the History of Alchemy and Chemistry (SHAC) belongs to the former category, while the Historical Group of the Royal Society of Chemistry represents the latter.

So, is there a future for self-education texts in chemistry? Electronic forms of learning are flourishing today, but the death of the printed book has been much exaggerated by futurologists. Certainly this has not happened in the humanities (which include the history of chemistry). The Covid-19 crisis has meant that traditional libraries have for a large part, been off-bounds from early 2020 and onwards, with distance-learning on screens becoming the norm for universities. But academic study is not the focus of this paper and attitudes taken by a curious public requires inspired guesses based on observable trends. Pure science does not hold a particularly high reputation amongst the general public, and in its place there appears to be no shortage of newly-authored, printed books which address how as-yet unresolved scientific problems challenge society, and how these will impact negatively upon life-styles and living conditions. Those requiring information rather than literary forms are more likely to turn to websites and television rather than printed paper.

Books dealing with the benefits of chemistry for today's public are rarer now than in the past, but then misery has always sold better than warmth. (People settling down to read a book on a long journey get more pleasure from being told about how terrible everything is, as newspapers have long known.) But for the minority who want to learn about serious science and its contemporary development, it is likely that electronic forms of information-provision will be the medium to which they turn. This is for various reasons. It is rapid to place before its audience, it is very easily accessible, it can be exceptionally rich in knowledge-provision, it can be entirely up-to-date. Moreover, it allows questioning, including one-to-one discussion with colleagues, some of whom may be geographically remote. A downside is that the rise of electronic communication through personal e-mails has as its concomitant the decline of traditional correspondence. This will have a major impact for chemistry historians of the future. E-mails are fugitive and tend to be archived only for official purposes. It is almost impossible to imagine how anything will endure in the way of those ideas, proposals, criticisms etc., at times when chemists corresponded with their colleagues, if key letters of the past had not been preserved. Our understanding of the thought-processes which led to major breakthroughs would simply not exist. The papers these chemists published rarely provide a substitute.

It is sensible to regard the printed book and electronic access to knowledge as complementary forms. Books are better at providing carefully considered opinions. They make authors think carefully about these opinions, knowing that once printed they are set in stone (or at least, in non-erasable ink). There are many stories about wild inaccuracies in certain electronic texts, and editorial checking and revision can be lax or non-existent. There can be an indiscipline in electronic forms which is rarer in books, where there is more financial and reputational commitment to producing accurate text for long-term usage. When Wikipedia gets it wrong, it can almost instantly be amended. Earlier versions disappear. Opinions expressed in Wikipedia are not ascribed to their authors. It can be revealing to compare earlier with later editions of printed books when changes have been introduced. If texts in printed form entirely disappear, much will be unavailable for future historians. The use to which they would have been put will change the nature of the history of chemistry for ever.

It must be appreciated that over the past couple of centuries there have been changing reasons why the public has wanted to learn about knowledge new to them. The mechanics who crowded in to the Andersonian Institution had different motives for understanding chemistry from those who were buying cheaply produced copies of the Teach Yourself series a century later, and very different from those readers anxious to find out reasons for climate change and what can be done about it. One thing can be said that is unlikely ever to change: the basic curiosity of serious-minded adults.

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About the Author

Robert G. W. Anderson made his way in UK national museums, first as a curator, then a director. He had graduated from Oxford in chemistry and for the whole of his career has published in the history of the subject. He won the Dexter Prize in 1986 and the Bunge Prize in 2016. He was President of the British Society for the History of Science, Chairman of the Society for the History of Alchemy and Chemistry, is a fellow of the Royal Society of Edinburgh, and an emeritus fellow of Clare Hall, Cambridge. Most recently, from 2016 to 2020, he has been President and CEO of the Science History Institute, Philadelphia.

MENDELEEV'S "PROBLEMS:" A MEANS TO ENGAGE STUDENTS AND TEACHERS IN THE HISTORY OF CHEMISTRY

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Abstract

As others have also noted, one means of engaging students and educators with the history of chemistry is to examine the errors by great historical chemists in their contemporary context. After providing very brief biographical background as well as a brief description of the path to the periodic table, three of Mendeleev's "problems" associated with his periodic table are described: 1) the "discrepancy" between the atomic weights of tellurium and iodine, 2) Mendeleev's difficulties in his initial acceptance of helium and argon, and 3) his hypothesis of the "super-light" inert gas atoms comprising the celestial ether.

Introduction

It is a real challenge to interest students, and even most educators, in the history of chemistry despite the statement by Oliver Sacks, renowned neurologist and author of the chemical memoir *Uncle Tungsten*: "Chemistry has perhaps the most intricate, most fascinating, and certainly most romantic history of all the sciences" (1). One solution might be to "humanize" the science. Providing dramatic details of the life of a chemist can be helpful. Yet another approach is to "catch" an iconic chemist making errors, a point eloquently made two decades ago (2), and to "teach the nature of science through scientific errors" (3). From a modern perspective, it is all too easy to point out the errors and misconceptions of even the most distinguished scientists, as theories and methodologies evolve. Value is only truly gained by understanding the contemporary context of these errors sometimes combined with some all-too-human foibles.

Dmitri Ivanovich Mendeleev is an iconic chemist (perhaps *the* iconic chemist). Indeed, the periodic table hangs in virtually every dedicated chemistry classroom and lecture hall, literally "the icon on the wall." Mendeleev has a very dramatic life story. His scientific "problems" reflect the absence of knowledge that awaited discoveries in future decades. But it is also clear that his magnificent development of the periodic law in 1869, initially handicapped somewhat his abilities to understand its occasional inconsistencies and extensions during his later years.

The details of Mendeleev's life will surprise most students (and many educators). The usual textbook photographs, dating from late in his life, suggest an almost biblical prophet. Indeed, his predicted discoveries of three new elements were prophetic. However, he also predicted the existence of elements never found (4) and classification of the lanthanides continued to confuse Mendeleev and others (5). As one might suspect, Mendeleev did not discover the periodic law in a dream (6). He was not a lone scientist, but active in industrial and governmental establishments. Perhaps the biggest surprise is that Mendeleev was never awarded the Nobel Prize in chemistry (7, 8).

The purpose of this brief article is to encourage the inclusion of history of chemistry in introductory courses. Its presentation is light and emphasizes three scientific problems: 1) Mendeleev's anticipated correction of the "reversal" of the atomic weights of iodine and tellurium, 2) Mendeleev's initial resistance to the discovery of the noble gases helium and argon, and 3) Mendeleev's hypothesis of atoms comprising the "universal ether."

A Very Brief Life of Mendeleev

Dmitri Ivanovich Mendeleev (February 8, 1834-February 2, 1907) (9) was born near Tobolsk in Siberia to Ivan Pavlovich Mendeleev (1783-1847) and Maria Dmitrievna Mendeleeva (née Kornilieva) (1793-1850) (10-13). He was the last of 14 children (9). To a comfortable family life came two disasters. Dmitri's father died in 1847 following years of illness and Maria was forced to work and resurrect the family glass factory in Tobolsk (13). The factory was destroyed by fire in 1848. Maria recognized Dmitri's intellectual gifts, sold her possessions and in 1849, with her youngest daughter Elizabeth also in tow, commenced a 2200-km journey to Moscow over the Ural Mountains. She failed in her attempt to enroll Dmitri in Moscow University and then traveled another 700 km to St. Petersburg (13). He was again denied entrance to the university but was admitted to the Chief Pedagogical Institute. The President of the Institute had been a fellow student of Dmitri's father. Fortunately, the Pedagogical Institute was located within the University of St. Petersburg and Dmitri had exposure to its scientists.

Exhaustion took its toll on Maria. She died in September 1850 from what is presumed to be tuberculosis just as sixteen-year-old Dmitri began his studies. Elizabeth also died a few months later. In a dedication to a paper published in 1887, Mendeleev wrote (13, 14):

> This investigation is dedicated to the memory of a mother by her youngest offspring. Conducting a factory, she could educate him only by her own work. She instructed him by example, corrected with love, and in order to devote him to science she left Siberia with him, spending her last resources and strength. When dying, she said, "Refrain from illusions, insist on work, and not on words. Patiently search divine and scientific truth."

He graduated from the Pedagogical Institute in 1856 and received its gold medal. His undergraduate thesis was defended in spring 1855 and his Masters thesis defended in September 1856 (10-12). Following graduation, Mendeleev became very ill and spent time in the milder climate in Crimea. He returned to St. Petersburg and was appointed a lecturer at the University. In 1859, the Russian government provided support for his study at Heidelberg University, which boasted famous chemists including Robert Bunsen (1811-1899) and Gustav Robert Kirchhoff (1824-1887). Bunsen and Kirchhoff would soon develop the spectroscope, the definitive detector of known and new chemical elements. Mendeleev declined the opportunity to work in Bunsen's laboratory, leading the great German scientist to resent the slight by the young Russian (15). In 1861, Mendeleev's textbook on organic chemistry won for him the prestigious Demidov Prize of the Petersburg Academy of Sciences. He married Feozva Nikitichna Leshcheva in 1862 and they had two children. Unhappily married from the start, he met Anna Ivanovna Popova in 1876, married her and divorced Lascheva in 1882. Anna and Dmitri had four children including twins. He became Doctor of Science in 1865 and was appointed Professor at the University of St. Petersburg in 1867. Teaching inorganic chemistry, Mendeleev began writing the textbook that would soon lead him to the periodic law.

The Paths to the Periodic Law

It is not the purpose of this brief paper to treat the development of the periodic law in any depth. Rather, it is worthwhile for students and teachers to briefly consider some questions:

1. What were the early foundations leading to the periodic law?

2. What drew Mendeleev to atomic weights as a critical organizing principle?

3. Why is Mendeleev, among worthy competitors, considered the father of the periodic table?

One of the earliest efforts to systematize chemical substances was by the French physician, Étienne François Geoffroy (1685-1752), who published the first affinity table in 1718 (Figure 1) (16). Column 9 represents substances having affinities for sulfur (at the top) ranging from highest (iron, Fe) to lowest (gold, Au). Although the chemical observations of the period were not always consistent, the match with the activity series of metals (reduction potentials relative to hydrogen) is striking: Fe^{2+} (–0.44 V, most difficult in the Column 9 series to reduce to the metal; therefore, metal most easily oxidized); Cu^{2+} (+0.34 V); Pb^{2+} (–0.13 V); Ag^{+} (+0.80 V); Hg^{2+} (+0.85 V); Au^{3+} (+1.52 V; metallic gold: hardest to oxidize). Tin was known before 1600 (*e.g.*, see Column

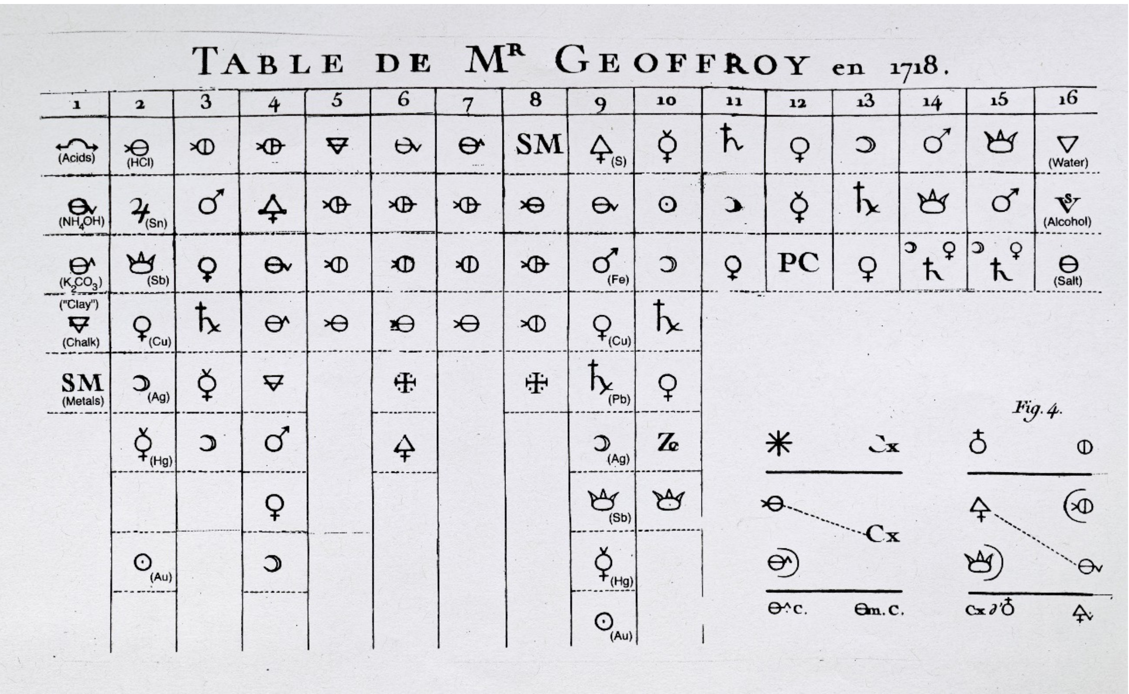


Figure 1. *A slightly modified version of Geoffroy's 1718 Table of Chemical Affinities (16). Photo courtesy of Richard P. Johnson.*

2) although not listed in Column 9. Its reduction potential (Sn^{2+}, –0.13 V) makes it significantly easier to reduce than iron. Thus, tin and copper, the elements of bronze, were easier to smelt (reduce their sulfide ores) than iron. The Bronze Age began around 3000 B.C. while the Iron Age began around 1200 B.C. A serious definition of a chemical element by Antoine Lavoisier would still be some seventy years in the future and the concept of atomic weights by John Dalton (1766-1844), an additional twenty years (Table 1). It is easy to see from our modern perspective the problems in this table arising from experimental errors, assumptions that gases such as hydrogen, nitrogen and oxygen are monoatomic rather than diatomic, and that the "ultimate particles" of water and ammonia were simply HO and NH. Dalton continued to hold these views well beyond the wide acceptance of more correct stoichiometries (17).

Table 1. Partial list of John Dalton's first table of "Atomic" Weights ("of the relative weights of the ultimate particles of gaseous and other bodies," 1805) (18)

Hydrogen	1
Azot (Nitrogen)	4.2
Carbone	4.3
Ammonia ("HN")	5.2
Oxygen	5.5
Water ("HO")	6.5
Phosphorus	7.2
Gaseous Oxide of Carbon (CO)	9.8
Sulphur	14.4
Sulphurated hydrogen ("HS")	15.4
Carbonic Acid (CO_2)	15.3
Carburetted hydrogen ("H_2C") from stag. water[a]	6.3

[a] Carburetted hydrogen (CH_4) isolated from bubbles arising from swamps (stagnant water) and reported by Alessandro Volta (1745-1827) in 1777.

The next twenty-five years following Dalton's atomic theory were critical ones for placing it on a more solid foundation. The gas laws provided greater understanding of the actual combination ratios to form molecules (19). Gay-Lussac demonstrated that two volumes of hydrogen gas combine with one volume of oxygen gas to form water (19). In 1811, Amedeo Avogadro (1776-1856) published his major work, now referred to as Avogadro's Law: under the same conditions of temperature and pressure, equal numbers of ultimate particles occupy equal volumes (19). Avogadro's nomenclature was confusing to those who read the work of this somewhat obscure academician. Its full impact would only be appreciated a half century later and truly set the stage for the periodic table. In 1814, André Marie Ampère (1775-1836) independently concluded that equal numbers of particles occupy equal volumes (19). In 1819, chemist Pierre Louis

Dulong (1785-1838) and physicist Alexis Thérèse Petit (1791-1820) demonstrated that "atomic heat," the product of specific heat (heat/mass) and atomic weight (mass/atom), was nearly constant for the 13 elements they reported (19).

Some credit William Prout (1785-1850) with the first numerical relationship between atomic weights (19). During 1815-1816 he compiled a table of densities of gaseous elements that were whole-number multiples of hydrogen. This suggested hydrogen as a sort of *primary material* constituting the mass of all other elements. As early as 1816-1817 Johann Wolfgang Döbereiner (1780-1849) observed that the atomic weight of strontium (accepted as 50 at the time), whose chemical properties were similar to calcium (27.5) and barium (72.5), was essentially the average of the other two (19). This *triad* might be considered as the first periodic relationship. During 1818-1819 Eilhardt Mitscherlich (1794-1863) related crystal structures and atomic composition (19). For example, phosphates and arsenates (*e.g.*, $Na_2HPO_4 \cdot 12H_2O$ and $Na_2HAsO_4 \cdot 12H_2O$) were found to be isomorphs, very similar crystal structures and analogous chemical compositions. Similar results were found for sulfates and selenates (*e.g.*, Na_2SO_4 and Na_2SeO_4). Today we recognize P and As in Group 15 (old VA) and S and Se in Group 16 (old VIA) of the modern periodic table. In 1818, Jöns Jakob Berzelius (1779-1848) published the most accurate known list of the atomic weights of 45 of the 49 elements known at the time (20). He extended this table with new discoveries in 1826 by which time there were 52 known elements. By 1829, other *triads* were recognized: lithium, sodium, potassium; sulfur, selenium, tellurium; manganese, chromium, iron. Döbereiner must have been elated that the atomic weight for the newly-discovered element bromine (1826), was the average of the atomic weights of chlorine and iodine. The isolation of fluorine was still some six decades away (but more on that later!). In 1826, Jean Baptiste André Dumas (1800-1884) developed a vapor density technique that established that gaseous elements, such as oxygen and chlorine, occur as diatomics, and that white phosphorus actually consists of P_4 molecules (19).

Efforts to systematize the elements continued during the 1840s and 1850s even with the uncertainties in atomic weights and uncertainties in stoichiometry. Thomas Graham (1805-1869) postulated eleven classes of elements based upon isomorphisms and chemical affinities (e.g., **First Class**: oxygen, sulfur, selenium, tellurium; **Fifth Class**: chlorine, iodine, bromine, fluorine) (21) which influenced Mendeleev's early thinking (22). In 1854, Josiah P. Cooke (1827-1894), Erving Professor of Chemistry at Harvard, published a paper relating atomic weights and chemical properties and providing a classification of elements into six series according to crystallographic systems. Here is Professor Cooke describing the need to better organize the chemical elements (23):

> In most elementary text-books on chemistry, the elements are grouped together with little regard to their analogies. Oxygen, hydrogen and nitrogen are usually placed first, and therefore together although there are hardly to be found three elements more dissimilar; again, phosphorus and sulphur, which are not chemically allied, are frequently placed consecutively, while arsenic, antimony, and bismuth in spite of their close analogies with phosphorus, are described in a different part of the book.

As well as to teach more effectively:

> As chemistry is usually taught, the properties of the members of this series, nitrogen, phosphorus, arsenic and antimony, as well as the composition and properties of their compounds, make up a large body of isolated facts, which, though without any assistance for his memory, the student is expected to retain. Certainly, it cannot be wondered at, that he finds this a difficult task. The difficulty can, however, be removed if after he has been taught that nitrogen… (reacts) with three equivalents of hydrogen to form NH_3, he is also told, that, if in these symbols of the nitrogen compounds he replaces N by P, As, or Sb, he will obtain symbols of similar compounds of phosphorus, arsenic or antimony.

The Impact of the Karlsruhe Conference of 1860

The uncertainties in the atomic weights of some elements and questions about stoichiometry prompted August Kekulé (1829-1896) to suggest the first major international meeting of European chemists, arguably the most important meeting in the history of chemistry (24). Kekulé and Charles-Adolph Wurtz (1817-1884) were the meeting organizers and Karl Weltzien (1813-1870), the host in the city of Karlsruhe, in September 1860. Among the 140 attending the meeting were chemists who would play major roles leading up to the periodic law: Jean Servais Stas (1813-1891, Belgium), Dumas (France), Julius Lothar Meyer (1830-1895, Germany), William Odling (1829-1921, England), Mendeleev (Russia) and Stanislao Cannizzaro (Italy). Cannizzaro's 1858 pamphlet (25) and presentation in Karlsruhe clarified Avogadro's half-century-old definition of atoms and molecules and

Figure 2. *Founders of the Russian Chemical Society. January 1868. Saint Petersburg; Among those standing: fifth from left, chemist-composer Alexandr Borodin; sixth from left, N. A. Menshutkin (1842-1907) who first presented Mendeleev's periodic law to the Russian Chemical Society on March 4, 1869; and second from right, Dmitri Mendeleev (age 34); seated, fourth from left, Vladimir V. Markovnikov (1833-1887, a favorite of organic chemistry students worldwide). Source: D. I. Mendeleev Museum-Archive (St. Petersburg State University) via Wikimedia Commons, https://commons.wikimedia.org/wiki/File:RFCS_1868.jpg (accessed 13 Aug. 2021).*

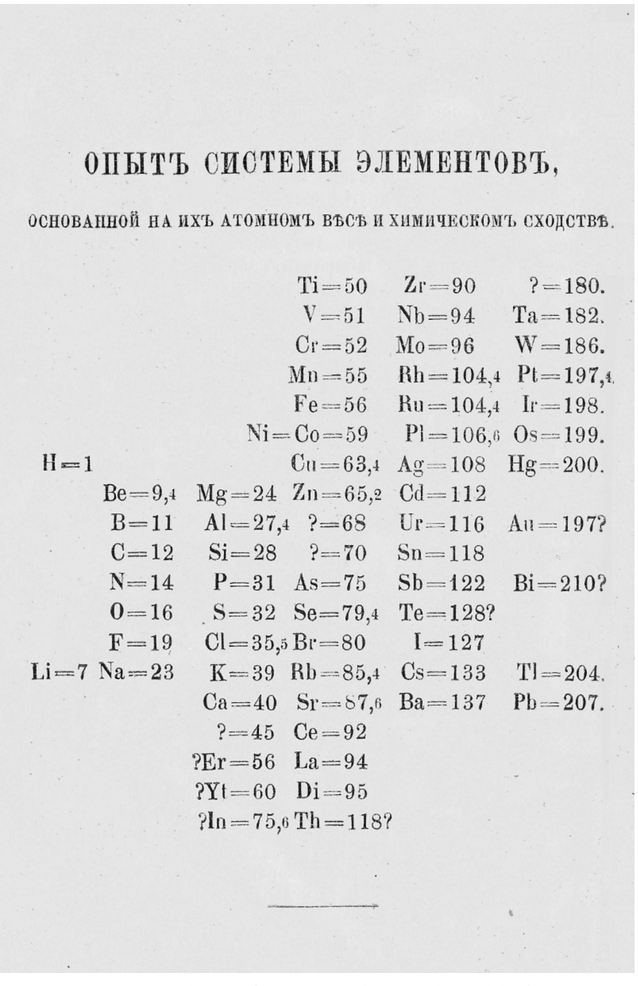
the relationship to Avogadro's law. Lothar Meyer was moved to comment (26):

> The scales seemed to fall from my eyes. Doubts disappeared and a feeling of quiet certainty took their place. If some years later I was able myself to contribute something toward clearing the situation and calming heated spirits no small part of the credit is due to this pamphlet of Cannizzaro.

Russia sent seven chemists to the Karlsruhe conference. The four-man St. Petersburg contingent included Mendeleev and Aleksandr Borodin (1833-1887). Borodin is most widely known as a composer, much more so than a chemist. However, he is a pioneer of the aldol condensation reaction taught to all first-year organic chemistry students today and an early pioneer in organofluorine chemistry (27). His most famous work was the opera "Prince Igor," composed over a seventeen-year period. It had to be completed posthumously by two great Russian composers, Nikolai Rimsky-Korsakov and Alexandr Glazunov (27). A scene from the opera, "Polovtsian Dances," still thrills audiences worldwide. The song "Stranger in Paradise" in the Broadway musical "Kismet," is derived from this musical scene (28). In Figure 2, we see Mendeleev and Borodin, two founding members of the Russian Chemical Society (today the Mendeleev Russian Chemical Society).

Returning from Karlsruhe, gifted minds turned toward understanding relationships among the elements with improved atomic weights and new creative energies (14). In 1862, A. E. Beguyer de Chancourtois (1819-1866), Paris École des Mines, proposed his "telluric helix" in which there were similarities between elements that fell on a line (14). John Alexander Reina Newlands (1837-1898) was an industrial chemist whose brief publications, in the *Chemical News*, beginning in 1863 were later collected into his 1884 book *On the Discovery of the Periodic Law and on Relations among Atomic Weights*. In 1864 he published an early version of his table of elements and commented that elements seven places apart frequently had similar properties (*e.g.*, nitrogen (sixth) and phosphorus (thirteenth)). In 1865 he described this as a "Law of Octaves" similar to music (*e.g.*, high C is the eighth note above middle C and twice the frequency) and he published a table of 62 elements highlighting chemical relationships. William Odling also published a table of elements in 1864, arranged in order of atomic weights and recognizing patterns in the atomic weights of elements having similar properties. Danish-born-and-educated Gustavus Hinrichs (1836-1923), published a helical table of the elements in 1867, while a faculty member at the University of Iowa (29). Probably the strongest claimant to some share of the credit for the periodic law was Julius Lothar Meyer. In 1868 he produced a table of elements meant to be included in a new edition of his textbook, but that table was never published. Intriguingly, his table not only left a gap in the carbon family between silicon and tin, it estimated an atomic weight (73) for the missing element that interpolated them. Meyer finally published his revised table of elements in 1870, very similar to Mendeleev's 1869 table although not claiming originality (14).

Initially, the organizing relationship between elements was valence (*e.g.*, Na_2O, CaO), so recently formalized by Edward Frankland (1825-1899) as well as Kekulé (30). But almost immediately it appeared quite reasonable to Mendeleev to build the periodic table according to increased atomic weight in combination with similarities in chemical and physical properties. At first glance it works quite well. But there were subtle inconsistencies that defied simple explanation. As reasonable as it appeared, almost a half-century later strict arrangement in accord with atomic weights was shown to be the incorrect approach. So why did Mendeleev settle on atomic weights for his ordinal arrangement of elements? Here Eric Scerri offers what he terms the "core philosophical idea of the periodic system" (30). He writes that Mendeleev differentiated *simple substances* and *elements*. Scerri employs an example to make his point. As we all enjoy teaching our students, the violently reactive, poisonous metal sodium combines with the violently reactive, poisonous gas chlorine to form table salt. Does sodium remain sodium, chlorine remain chlorine and the two somehow display affinity and combine in salt? Metallic sodium and gaseous chlorine are, according to Mendeleev, the familiar *simple substances* that exist prior to their combination. An *element* is, however, a more abstract thing and exists in some form in the compound. Thus, sodium is no longer a highly reactive, toxic metal and chlorine no longer a highly reactive toxic gas when combined in table salt. The chemical properties of these two simple substances are not invariant but change drastically in compounds. In contrast, all experimental data support the view that from element to compound to new compound, atomic weights remain invariant. Therefore, using this invariant, intrinsic property to order and classify the elements appears to have been a most sensible approach. Figure 3 is an image of Mendeleev's the periodic table printed in the first edition of *Osnovy Khimii* (31). P. A. Druzhinin makes the compelling case for this being the first printed version (32).



ОПЫТЪ СИСТЕМЫ ЭЛЕМЕНТОВЪ,

ОСНОВАННОЙ НА ИХЪ АТОМНОМЪ ВѢСѢ И ХИМИЧЕСКОМЪ СХОДСТВѢ.

			Ti=50	Zr=90	?=180.
			V=51	Nb=94	Ta=182.
			Cr=52	Mo=96	W=186.
			Mn=55	Rh=104,4	Pt=197,4.
			Fe=56	Ru=104,4	Ir=198.
			Ni=Co=59	Pl=106,6	Os=199.
H=1			Cu=63,4	Ag=108	Hg=200.
	Be=9,4	Mg=24	Zn=65,2	Cd=112	
	B=11	Al=27,4	?=68	Ur=116	Au=197?
	C=12	Si=28	?=70	Sn=118	
	N=14	P=31	As=75	Sb=122	Bi=210?
	O=16	S=32	Se=79,4	Te=128?	
	F=19	Cl=35,5	Br=80	I=127	
Li=7	Na=23	K=39	Rb=85,4	Cs=133	Tl=204.
		Ca=40	Sr=87,6	Ba=137	Pb=207.
		?=45	Ce=92		
		?Er=56	La=94		
		?Yt=60	Di=95		
		?In=75,6	Th=118?		

***Figure 3**. Mendeleev's first printed periodic table from 1869* Osnovy Khimii *(*Principles of Chemistry*) (31) (from the collection of Gregory S. Girolami and Vera V. Mainz).*

Mendeleev's Successful Predictions of New Elements

The unique triumph of Mendeleev's periodic law was his daring prediction of three unknown elements corresponding to gaps in the table: *ekaboron*, *eka-aluminum* and *ekasilicon* including the prediction of their physical and chemical properties (*eka* = "one" in Sanskrit implying one beyond). Partington comments: "The publications of Lothar Meyer in 1870 and Mendeléeff in 1871 attracted very little interest" (14). This changed abruptly when Paul Émile Lecoq de Boisbaudran (1838-1912), working in the laboratory of Wurtz in Paris, discovered eka-aluminum (gallium) via spectroscope in 1875 (33). In 1879, the Royal Society awarded Lecoq de Boisbaudran the Davy Medal (named for the great early nineteenth century chemist Humphry Davy, 1778-1829) for this ground-breaking discovery. Lars-Fredrik Nilson (1840-1899), working in Uppsala Sweden, reported ekaboron (scandium) in 1879 (34). In 1882, the Royal Society presented the Davy Medal jointly the Mendeleev and Meyer ("For the discovery of the periodic relations of the atomic weights"). In the preface to his aforementioned 1884 book, Newlands states (35):

> Having been the first to publish the existence of the periodic law more than nineteen years ago, I feel, under existing circumstances, compelled to assert my priority in this matter.

Among his claims, Newlands mentions his "Prediction of the atomic weight of missing elements, such as the missing element of the carbon group = 73, since termed eka-silicium by M. Mendelejeff" (35). Clemens Alexander Winkler (1838-1904), in Freiberg Germany, reported ekasilicon (germanium) in 1886 (36). Its atomic weight is 73. In 1887, Newlands received the Davy medal from his fellow countrymen ("For his discovery of the periodic law of the chemical elements").

Before moving on, let us spend a moment on the topic of "simultaneous discoveries" in chemistry. Perhaps the classic is the discovery of oxygen. It is popularly credited to Englishman Joseph Priestley (1733-1804) who made his discovery in 1774 and published first in 1775 (37). However, the discovery of "fire air" was made first in Uppsala, Sweden by Carl Wilhelm Scheele (1742-1786) somewhere between 1770 and 1773, but publication was delayed until 1777 (38). Priestley was unaware of Scheele's discovery (38). Both Priestley, who named the newly-discovered gas "dephlogisticated air," and Scheele were proponents of the phlogiston theory that would soon be totally discredited by Lavoisier. Since the purpose of the present article is to stimulate interest in incorporating history of chemistry into the introductory course, let us "give a plug" to the play *Oxygen*, authored by the distinguished chemists Carl Djerassi and Roald Hoffmann, authors of novels, plays and poetry (39). They imagine the first "retro-Nobel Prize" and a dramatic debate among a modern committee about the appropriate awardee(s) (Lavoisier, Priestley or Scheele or some combination). It is instructive and fun for students (and teachers) to perform the play in full or even in part in class. Perhaps an even more striking case of simultaneous discoveries is the near-simultaneous publications in 1874 of the tetrahedral carbon by Jacobus Henricus van't Hoff (1852-1911) and Joseph Achille Le Bel (1847-1930) who knew each other while working in close proximity in Wurtz's Paris laboratory. Their papers took very different approaches reaching similar conclusions and were developed totally independently (40). In the case of the periodic table, the Karlsruhe conference stimulated the contributions to the periodic law that almost immediately followed. For van't Hoff and Le Bel, one can argue that the advancement of structural organic chemistry during the prior two decades set the stage for the next logical steps climbed virtually simultaneously by two young chemists. Let us also note Jeffrey Seeman's discussion, including a very thorough taxonomy, of "Multiple Simultaneous Independent Errors" in contrast to "Multiple Simultaneous Independent Discoveries" (41). He provides the example of two research groups independently publishing the same incorrect structure for the newly-discovered organometallic molecule ferrocene. Indeed, Scheele's and Priestley's adherence to phlogiston theory to explain combustion, even as they each discovered oxygen, is another example.

On June 4, 1889, Mendeleev delivered the Faraday Lecture before Fellows of the Chemical Society in the Theatre of the Royal Institution (42). He lauds the contributions by Cannizzaro at Karlsruhe that clarified the difference between atomic and equivalent weights and dismisses some details of Newlands' periodic table, noting for example, that some of Newlands' octaves had ten elements with two elements occupying the same space (*e.g.*, Co and Ni). Mendeleev admits to not knowing the physical origin of atomic weights but dismisses Prout's revival of the ancient Greek concept of a *prima materia*, noting that while some had assigned the 0.0005875 mm line in the sun's corona to a new element ("helium"), others equated it to the primary material. Mendeleev also rejects "helium" since it was not observed outside the sun's flares; he considered it an artifact of high temperature and pressure on the spectrum of a solar element, perhaps hydrogen. Proudly referring to the discoveries of gallium, scandium and most recently germanium, Mendeleev declared (42):

> When, in 1871, I described to the Russian Chemical Society the properties, clearly defined by the periodic law, which such elements ought to possess, I never hoped that I should live to mention their discovery to the Chemical Society of Great Britain as a confirmation of the exactitude and the generality of the periodic law.

He then went on to predict the existence and, in considerable detail, the physical and chemical properties of "dvi-tellurium" (*dvi* = two in Sanskrit). The element in question was ultimately radioactive polonium, discovered by Marie and Pierre Curie in 1898 (43). (Radioactivity was unknown in 1889.)

Solutions to Mendeleev's Confusion on "Inverted" Atomic Weights: Isotopes and Atomic Numbers

Among the small discrepancies that still existed among atomic weights even after the superb experimental work by Stas, the anomaly between tellurium and iodine depicted in Table 2 was particularly vexing to Mendeleev. He clearly recognized the appropriate placement of iodine below bromine and tellurium below selenium despite the significant reversal in atomic weights. Mendeleev was confident that future experimental analyses would place these elements in their proper order of atomic weights.

Prout's rule, simple and attractive as it was, led to considerable confusion once it was more closely examined. In Berzelius' 1826 table, the atomic weight of chlorine was listed at 35.4 (hydrogen = 1). Thomas Thomson (1773-1852), a respected chemist, published a table of atomic weights in 1825, which were, conveniently, whole number multiples of hydrogen including chlorine which he rounded up to 36. To this, Berzelius wrote (19):

> Much of the experimental part, even of the fundamental experiments, appears to have been made at the writing desk; and the greatest civility which his contemporaries can show its author, is to forget that it was ever published.

Working with Josiah Cooke at Harvard, his student Theodore William Richards (1868-1928) was able to very carefully check and slightly modify Stas's atomic weights. Cooke and Richards demonstrated that the accurate atomic weight ratio of oxygen to hydrogen was 15.95, not 16.00 (44). Richards would join the Harvard faculty, later determining that cobalt is indeed heavier than nickel (45, 46) despite the seeming anomaly (Table 2).

Today we recognize that one major problem for Mendeleev was the absence of knowledge of isotopes during his lifetime (see Table 2). During 1906 and 1907, the year Mendeleev died, a number of researchers investigated the elements produced by radioactive decay (47). In 1913, Frederick Soddy (1877-1956), one of the principal researchers in this newly-emergent field of radiochemistry, defined isotopes as examples of the same element differing only in atomic weight (47). Soddy would win the 1921 Nobel Prize. Richards, continuing his careful redetermination of atomic weights discovered that naturally-occurring lead and lead derived from radioactive decay were isotopes (47). He won the Nobel Prize in Chemistry in 1914, the first American so honored. In 1919, Francis William Aston (1877-1945), with his early mass spectrometer (1922 Nobel Prize in chemistry), an instrument that separates positive ions based upon mass/charge differences, discovered two isotopes of neon: the first identification of non-radioactive isotopes (47). The underlying difference between isotopes was the neutron which would await James Chadwick's (1891-1974) discovery in 1932 (48) (1935 Nobel Prize in Physics).

Table 2. Problems in placing elements in strict order of atomic weight (modern atomic weights listed based upon ^{12}C).

ELEMENTS SEEMINGLY OUT OF ORDER:

15 (VA)	16 (VIA)	17 (VIIA)
As	Se	Br
74.92	78.97	79.90
Sb	Te	I
121.76	**127.60**	**126.90**

9 (VIII)	10 (VIII)
Co	Ni
58.93	**58.69**

Returning to the seeming anomaly between iodine and tellurium, while the isotope ^{127}I comprises virtually 100% of the naturally-occurring element, there are six significant naturally-occurring tellurium isotopes with the heaviest, ^{130}Te, comprising 34.1%. Cobalt is virtually 100% ^{59}Co, while the lightest isotope, ^{58}Ni, is the most abundant (68.1%) of nickel's five major isotopes.

Henry G. J. Moseley (1887-1915) studied the series of certain X-rays (termed K_α) emitted from different metallic anticathodes (48). He observed a near-perfect linear relationship when plotting the square root of their frequencies versus simple ordinal numbers (1, 2, 3, …). These *atomic numbers* determine the true order of elements in the periodic table. Thus, the final clarification of Mendeleev's worries about inconsistencies in order occurred not long after his death. Moseley, who volunteered to fight in the First World War, was killed at the age of 28 in the disastrous Battle of Gallipoli (48).

Mendeleev's Helium and Argon Problem

Mendeleev's skepticism about the discovery of helium was noted earlier. Observed close to the doublet of sodium D-lines (49), the new solar emission reported by Joseph Norman Lockyer (1836-1920) was designated D_3. Lockyer and Frankland unsuccessfully attempted to reproduce the line by putting known elements under extreme conditions. Although these investigators did not formally attribute the line to a new element, such an explanation circulated widely among chemists and astronomers (50). The name "helium" (after the Greek *helios* = sun) is attributable to Lockyer (51). Part of Mendeleev's problem with helium was that he could not envision a place for this lone element in his periodic table. But the other part was that there were no earthly samples that could be checked for the D_3 line spectroscopically or analyzed for physical and chemical properties.

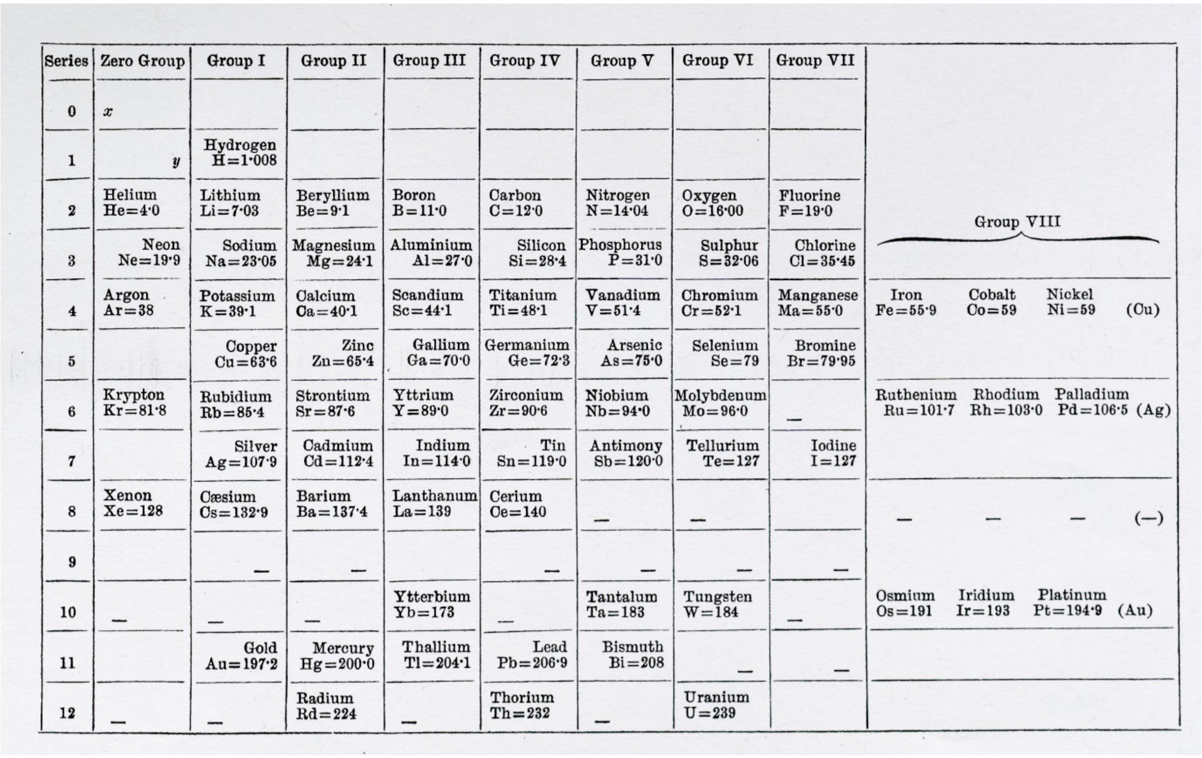
Precise measurement of atomic mass occupied many scientists during the second half of the nineteenth century and into the early twentieth century. John William Strutt (1842-1919, Lord Raleigh), a physicist, demonstrated even greater precision than Cooke and Richards with an O/H atomic weight ratio of 15.869 (44). He then set his sights on nitrogen, the most abundant element in the earth's atmosphere and encountered a conundrum. The density of atmospheric nitrogen was 0.535 percent greater than that of nitrogen obtained from pure chemical compounds. He communicated with chemist William Ramsay (1852-1916) who carefully ran atmospheric air through a series of chemical traps, removing CO_2 and H_2O using soda lime and Fe_2O_3, followed by red hot copper to remove O_2 and finally bright red hot magnesium to remove N_2. The remaining unreacted gas accounted for nearly 1% of the atmosphere, with a density twenty times that of H_2. Particularly unsettling, the ratio of specific heats at constant pressure to constant volume (C_P/C_V) was consistent with a monoatomic gas, the only precedent being mercury vapor. Rayleigh and Ramsay announced their findings in August 1894, published their discovery in the *Philosophical Transactions of the Royal Society* in 1895 and their Hodgkin's Prize-winning paper was published by the Smithsonian Institution in 1896 (52). This paper even acknowledged Henry Cavendish (1731-1810) who, in 1785, isolated a totally unreactive bubble comprising 1/120 of his original air sample. Over a century after Cavendish, the gas was named "Argon" (Greek = "inactive") (53). Rayleigh received the 1904 Nobel Prize in Physics and Ramsay the 1904 Nobel Prize in Chemistry.

Mendeleev was very discomfited by this discovery. There was apparently no place in the periodic table for argon. Assuming it really was monoatomic, its atomic weight might somehow squeeze it between potassium (39) and calcium (40) with chemistry totally unlike these metallic elements. Very skeptical about the discovery, Mendeleev postulated that argon was very possibly N_3 (molecular weight 42). Although the oxygen allotrope ozone (O_3) was known, it was far more reactive than the common atmospheric gas. It would seem something of a stretch to assume that a putative nitrogen allotrope (N_3) would be even less reactive than N_2 and that the atomic weight of a totally unreactive gas could be in error by some five percent.

As early as 1888, mineralogist William F. Hillebrand (1853-1925) of the U.S. Geological Survey discovered that minerals containing uranium, such as cleveite, included tiny quantities of an unreactive gas. In January 1895 the British mineralogist Henry Miers wrote to Ramsay about Hillebrand's work, and Ramsay purchased some cleveite intending to analyze what gas might be trapped within. In March 1895, Ramsay and William Crookes (1832-1919) demonstrated that its emission spectrum (D_3 line) corresponded to the solar element and thus, helium was indeed an earthly element (54). In 1904, the cleveite mystery was solved when Ramsay and Soddy established that α-particles emitted from radium were, effectively, helium.

Not long after the discoveries of argon and helium, Ramsay applied newly-discovered techniques for liquifying air and in 1898, with his graduate student Morris William Travers (1872-1961), detected and characterized neon (Ne), krypton (Kr) and xenon (Xe). Here is Travers writing about the first detection of neon (55):

> We each picked up one of the little direct-vision spectroscopes which lay on the bench. But this time we had no need to use the prism to decide whether or not we were dealing with a new gas. The blaze of crimson light from the tube told its own story, and it was a sight to dwell upon and never forget.



Series	Zero Group	Group I	Group II	Group III	Group IV	Group V	Group VI	Group VII	Group VIII
0	*x*								
1	*y*	Hydrogen H=1·008							
2	Helium He=4·0	Lithium Li=7·03	Beryllium Be=9·1	Boron B=11·0	Carbon C=12·0	Nitrogen N=14·04	Oxygen O=16·00	Fluorine F=19·0	
3	Neon Ne=19·9	Sodium Na=23·05	Magnesium Mg=24·1	Aluminium Al=27·0	Silicon Si=28·4	Phosphorus P=31·0	Sulphur S=32·06	Chlorine Cl=35·45	
4	Argon Ar=38	Potassium K=39·1	Calcium Ca=40·1	Scandium Sc=44·1	Titanium Ti=48·1	Vanadium V=51·4	Chromium Cr=52·1	Manganese Ma=55·0	Iron Fe=55·9 Cobalt Co=59 Nickel Ni=59 (Cu)
5		Copper Cu=63·6	Zinc Zn=65·4	Gallium Ga=70·0	Germanium Ge=72·3	Arsenic As=75·0	Selenium Se=79	Bromine Br=79·95	
6	Krypton Kr=81·8	Rubidium Rb=85·4	Strontium Sr=87·6	Yttrium Y=89·0	Zirconium Zr=90·6	Niobium Nb=94·0	Molybdenum Mo=96·0	—	Ruthenium Ru=101·7 Rhodium Rh=103·0 Palladium Pd=106·5 (Ag)
7		Silver Ag=107·9	Cadmium Cd=112·4	Indium In=114·0	Tin Sn=119·0	Antimony Sb=120·0	Tellurium Te=127	Iodine I=127	
8	Xenon Xe=128	Cæsium Cs=132·9	Barium Ba=137·4	Lanthanum La=139	Cerium Ce=140	—	—		— — — (—)
9		—	—		—	—	—	—	
10	—	—	—	Ytterbium Yb=173	—	Tantalum Ta=183	Tungsten W=184	—	Osmium Os=191 Iridium Ir=193 Platinum Pt=194·9 (Au)
11		Gold Au=197·2	Mercury Hg=200·0	Thallium Tl=204·1	Lead Pb=206·9	Bismuth Bi=208	—	—	
12	—	—	Radium Rd=224	—	Thorium Th=232	—	Uranium U=239		

***Figure 4**. Mendeleev's hypothesis of element "*x*" comprising the "celestial ether" (56). Photograph courtesy of Richard P. Johnson.*

Clearly, a new chemical family, a group of inert gases, existed and did indeed fit at the end of the periodic table. But which end: left or right? The right-hand side would place the group next to other non-metals (the halogens, Group VII) including two gases. Placement on the left-hand side would have them neighboring the alkali metals, but also hydrogen (Group I). Since the new gases were zero-valent, placing them in Group Zero to the left of Group I would appear to make some sense although this led to other problems.

Is The Celestial Ether Composed of Inert Gas Element "*x*" (Atomic Weight 0.00000096 or less)?

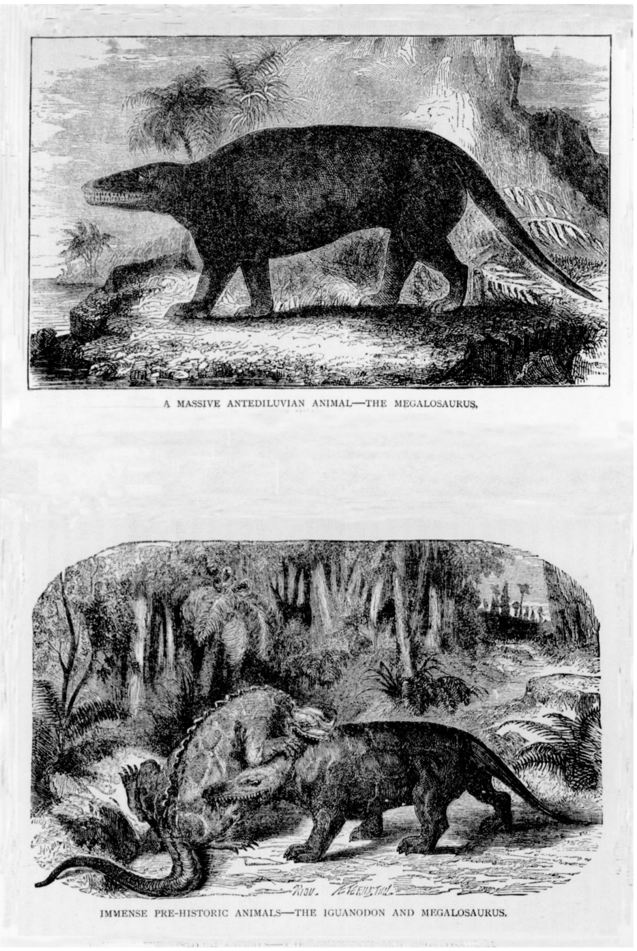
The wave nature of light was fully established in the nineteenth century. Just as air is required to carry sound waves, could an all-surrounding "fabric," an invisible "celestial ether" be required to carry light waves? Since the earth presumably moves through this stationary ether, the velocity of light should vary when measured in different directions. Physicist Albert Abraham Michelson (1852-1931) began an investigation in Germany in 1880-81 and, working in the United States, with chemist Edward W. Morley (1838-1923). In 1887, they discovered that the velocity of light is independent of direction, a crucial indicator that there is no "celestial ether." Michelson received the 1907 Nobel Prize in physics. Nevertheless, Mendeleev remained a believer and in 1902 published a pamphlet in Russian [1904 English translation, *An Attempt Towards A Chemical Conception of the Ether* (56)]. By this time, fully accepting the inert gases (Group Zero), he conceived of unimaginably light inert gas atoms capable of fully penetrating matter (57). Instead of the interpolating logic of Döbereiner, nearly ninety years earlier, Mendeleev used extrapolation on Group Zero. Since Helium could be classified in Period 2 Group Zero (Figure 4), there should be an element ("*y*"), the putative "coronium" (58, 59), in Period 1 Group Zero. Its atomic weight extrapolated to 0.4 (hydrogen = 1.0), clearly too massive for atoms of the celestial ether. So, Mendeleev invoked element "x," in Period Zero Group Zero, as the element comprising the celestial ether. He estimated its atomic mass as 0.00000096 or much lighter (hydrogen = 1).

Here is Mendeleev explaining his hypothesis of atoms lighter than hydrogen with reference to his original (1869) periodic table (56):

> …although I had a vague notion that hydrogen might be preceded by some elements of less atomic weights,

> I dared not put forward such a proposal, because it was purely conjectural, and I feared to injure the first impression of the periodic law by its introduction.

How does one come to grips with a theory that one might even consider "crank science"? Mendeleev was so strongly wedded to his periodic table, validated by his amazing predictions of new elements, that he may have misled himself into "cramming" ether theory into his periodic law (60). One can imagine an analogy here. Books depicting dinosaurs in the late nineteenth century included pictures like those in Figure 5. What were the origins of these strange images? Fossils are not discovered neatly arranged in skeletons. Rather, once discovered and typically incomplete, they were assembled during the nineteenth century according to contemporary knowledge and experience. The largest land-roaming carnivores were bears. So why not assemble megalosaurus to look like a bear? In the case of the vegetarian iguanodon, also assume a four-legged beast. Today we know that both these dinosaurs were bipedal and mostly vertical. Just as these constructions involved "cramming" fossil bones into pre-conceived skeletal configurations, so too did Mendeleev fall into the trap of "cramming" ether theory into the periodic law.



A MASSIVE ANTEDILUVIAN ANIMAL—THE MEGALOSAURUS.

IMMENSE PRE-HISTORIC ANIMALS—THE IGUANODON AND MEGALOSAURUS.

***Figure 5**. Nineteenth century depictions of dinosaurs formed by "cramming" fossil remains into pre-conceived models of large land animals (60).*

No Nobel Prize for Mendeleev: Strange Goings-On in Sweden

It does come as a disappointment and indeed almost a shock to learn that Mendeleev did not win a Nobel Prize. The details (61) are not pretty. When Nobel prizes were first awarded in 1901, they were intended to recognize recent research. However, the 1905 Nobel Prize in chemistry was awarded to Adolph von Baeyer (1835-1917) in recognition of his work on dyes and other contributions to organic chemistry significantly accomplished in the 1860s. Invoking a rule that allowed recognition of older advances achieving importance in recent times cleared the way for Baeyer and opened the door in 1906 for Mendeleev. Although the periodic law was almost forty years old, more recent discoveries, including the predicted elements and comfortable fit of the noble gases into the periodic table, satisfied these criteria. In 1905, Mendeleev and Ferdinand Frédéric Henri Moissan (1852-1907), who isolated fluorine developed the electric furnace, were the most significant competitors to Baeyer. In 1906, despite more previous nominations and votes for Moissan, the five-person chemistry Nobel committee voted four-to-one in favor of Mendeleev. However, the dissenting vote, Peter Klason, Royal Institute of Technology in Stockholm, argued strenuously against this choice. One line of argument, incredibly enough, was that the periodic table was already in use worldwide-effectively "old news." The argument was also made that the periodic law could not have been developed without Cannizzaro's clarifications of Avogadro's law. Therefore, a Nobel awarded to Mendeleev must be shared with Cannizzaro. However, since Cannizzaro had not been nominated earlier in 1906 for the prize, he was ineligible for the award that year. The Swedish Academy, which would normally "rubber stamp" the recommendation of the chemistry committee, added four distinguished chemists to the committee, hoping for clear consensus. The augmented committee proceeded to vote five to four in favor of Moissan who duly received the 1906 Nobel Prize. There was another major obstacle between Mendeleev and the Nobel Prize: Svante Arrhenius (1859-1927, 1903 Nobel Prize in chemistry). Mendeleev had been critical of the ionic theory of Arrhenius and this earned him a degree of antipathy from the great Swedish scientist (8). In early 1907, Mendeleev died. Nobel prizes are not awarded posthumously. As the authors note (61), October 27, 1906, when the committee voted for Moissan "…is not one of its more glorious days." How ironic that Moissan died in 1907, having just been awarded the 1906 Nobel Prize, while Mendeleev died in 1907 having just missed the 1906 Nobel Prize. There is some poetic justice in that among the names cited earlier, most closely associated with the development of the periodic table, there is only the eponymous element, Mendelevium (Md, Z = 101), and it precedes Nobelium (No, Z = 102).

Conclusions

There is enough content in introductory chemistry courses to discourage adding history of chemistry. However, teaching how science is "done," beyond the formulaic "scientific method," is really critical, especially at a time when the process itself is under populist pressure. It is important to teach young scientists that doing science is not the same as learning settled science. In the former, the right answers are not known (or at least not yet known). Scientists at the forefront of new knowledge often propose explanations that are later seen to be incorrect or inadequate. As inspiring as is the history of discovery that led to the science taught in textbooks (such as the periodic table), it is also important for students to see that not all of the work of even the most successful scientists stands the test of time. Mendeleev is hardly alone among scientists of the past about whom this point can be made; he is just one of the most likely to be mentioned in an introductory textbook.

Moreover, there is much to be said for "hands-on" learning. Performing the brief "masque" by the Lavoisiers in the play *Oxygen* (39) is one opportunity. The meeting between Werner Heisenberg and Niels Bohr, concerning the atomic bomb, in the play *Copenhagen* offers another opportunity explore the roles of scientists as human beings (62). And there was surely enough drama at the Karlsruhe conference to stimulate academic research and student performance.

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Arthur Greenberg was born in Brooklyn, New York and received his Ph.D. in chemistry from Princeton University (1971). He retired in May 2021 following twenty-one years at the University of New Hampshire as Dean of Engineering and Physical Sciences (2000-2005) and Professor of Chemistry (2000-2021).

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ARCHAEOLOGICAL CHEMISTRY: PAST, PRESENT, FUTURE

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Abstract

The ACS Division of the History of Chemistry (HIST) is the sponsor of possibly the largest and most comprehensive collection of volumes specifically on the topic of Archaeological Chemistry (AC) in the world. While it might be difficult to measure this content against other collections, the oeuvre consists of nine volumes published between 1974 and 2020. This paper will detail the past, consisting of the contents of the first seven volumes published between 1974 and 2007; the present, consisting of the contents of the last two volumes published in the second decade of the 21st century; and the future, consisting of projections and consultations with currently practicing archaeological chemists.

Introduction

"Archaeological chemistry is a topic which, when mentioned in a general public gathering, makes heads turn, eyes brighten, smiles burst forth and questions emerge" (1). This, the opening sentence of the most recently published HIST volume on archaeological chemistry, has held true for the entire 47-year history of this series.

The symposia, followed by volume publication, and held on average about every six years since 1973, have been co-sponsored by HIST's Subdivision of Archaeological Chemistry since 1974, although four other symposia (2) preceded those which are now contained in the nine published volumes attributed to HIST's direct sponsorship. Many of the subdivision's members are associate members, which means that they are not ACS members due to ineligibility, international status, or practice of a related discipline. But they come out in droves for this long-awaited event, lending a visibility and camaraderie to both HIST and to the ACS that can only be described as enviable. As a collection, the nine volumes have traced the development of archaeological chemistry from an emphasis on excavations, instrumental methods, and interdisciplinary coverage to an emphasis on cultural context, combined analytical techniques and statistics to interpret results and discoveries.

A Little Bit of History

"In the beginning" archaeological chemistry could be defined as the application of chemistry to archaeological materials. According to Oxford archaeological chemist A. Mark Pollard, the first published chemical analyses of archaeological bronzes in 1777 by Johann Christian Wiegleb (1732-1800) marks archaeological chemistry as one of the first disciplines to make use of gravimetric chemistry (3). This established relationship between archaeology and the analytical sciences continued with the work of Martin Heinrich Klaproth (1743-1817) who applied analytical techniques to the composition of some Greek and Roman coins. Other eminent scientists

Table 1. Summaries of the Prefaces of Volumes I through VII of the Archaeological Chemistry Series (1974-2007)

Volume	Preface Summary
AC I: 1974 C. Beck, Ed. (6)	AC is becoming a discipline in its own right. Data developed reveals patterns useful for determining context and meaning of archaeological data. It defines artifact analysis as the particular province of chemists.
AC II: 1978 G. Carter, Ed. (7)	AC is a maturing field showing signs of vigorous growth. Its avowed purpose is to "deduce history from the analysis and investigation of artifacts." It defines data reporting procedures, sample handling procedures, and standards definitions as areas to be addressed.
AC III: 1984 J. B. Lambert, Ed. (8)	This volume emphasizes how analytical instrumentation provides mainstream contributions to our understanding of archaeological artifacts and how advanced methods have made possible entirely new applications in archaeology, for example, to date objects as well as analyze them.
AC IV: 1989 R. O. Allen, Ed. (9)	This volume expands the field of AC to encompass not only a better understanding of the past, but also an ability to project a future. It also views AC as inherently multidisciplinary.
AC V: 1995 M. V. Orna, Ed. (10)	This volume emphasizes how coupling some instrumental methods in tandem allows for expanding the scope of the kinds of materials that can be examined as well as their increased sensitivity to ultratrace levels.
AC VI: 2002 K. A. Jakes, Ed. (11)	Emphasis in this volume is on nondestructive methods, ability to infer human behavior through analysis and new developments in age dating.
AC VII: 2007 M. D. Glascock, R. J. Speakman and R. S. Popelka-Filcoff, Eds. (12)	This volume continues the themes of the past six volumes, again putting emphasis on the broad interdisciplinarity of the field.

dedicated to the scientific examination of antiquities over the course of the 18th and 19th centuries were Humphry Davy (1778-1829), Jöns Jakob Berzelius (1779-1848) and Marcelin Berthelot (1827-1907) (4).

Shedding light on the past by means of scientific examination received great impetus when major museums began to establish laboratories for that purpose on their premises in the early 20th century. For example, the work of Alexander Scott (1853-1947) gave rise to the world-renowned laboratories of the British Museum. While museums were mainly concerned with examination of their own holdings, many university laboratories in departments of archaeology, anthropology and chemistry found ample work by examination of materials from excavations worldwide. The modern field of archaeological chemistry arose during the first 30 years following World War II as a result of the development of instrumental methods of inorganic analysis which made it possible to cultivate new areas in archaeological chemistry. However, the task of the archaeological chemist has become more complex than ever over the past half-century. Gone are the days of trying to answer the simple questions of "what?," "when?" and "where?" At one time, archaeological chemistry may have been considered the domain of analytical chemists turned "amateur archaeologists." However, effective work in this area demands being attuned to the increasingly multidisciplinary nature of the field along with the necessity of advanced instrumentation, ability to handle and interpret large databases of information and meaningful collaboration among many different kinds of workers (5). In the final section of this paper, we will hear directly from eminent practicing archaeological chemists as to how they perceive the future of this developing discipline. But first we must take a peek at the past and the present as discerned from the contents of the HIST AC collection.

Archaeological Chemistry Past

Admittedly, each of these volumes was a snapshot of what was going on in an emerging field at a particular moment in time. As such, we are dealing with a very small

Table 2. Subject Matter by Chapter Addressed by All Nine AC Volumes (1974-2020)

Subject Matter	**I 1974**	**II 1978**	**III 1984**	**IV 1989**	**V 1995**	**VI 2002**	**VII 2007**	**VIII 2013**	**IX 2020**
Number of Chapters	13	20	22	27	31	15	28	23	18
Number of Pages	254	389	487	508	459	259	571	472	509
Perspectives, General, Techniques	2	5			4	4	6	7	1
Role of Chemists in AC				1					
History of AC								1	
Educational Applications									3
Building Materials, Minerals, Materials Science							3	3	6
Ceramics, Glass, Pottery	4	4	4	4	2	5	7		
Colorants, Inks	1		3		3	1	1	4	6
Diet Analysis						1			
Fibers				5	7				
Isotope Analysis, Dating								3	
Lithic Materials, Soils, Residues, Bone, Shell	1		6	3	10		3	5	
Metals	5	5	3	7	3	1	5		
Nucleic Acids Analysis					2				
Organic Materials		6	6	7		3	3		2

slice of a very large pie and therefore, any conclusions drawn must necessarily be taken with a grain of salt. The topics addressed reflect the specific interests of the participants. Taken together, they may not represent the entire body of archaeological chemists.

One way of getting a taste of each volume is to read the preface which gives an overview of the discipline and at the same time summarizes the work in the individual chapters. Table 1 presents précis of the first seven of the volumes which, altogether, describe "Archaeological Chemistry Past."

From the content of these prefaces, it is possible to discern an evolution from an emerging to a mature discipline with a clear direction regarding subject matter, interpretation, methodology, and interdisciplinary nature. What becomes apparent from the preface of volume VII is that the growth in self-knowledge of the discipline has become asymptotic—tapering off to repeat the themes of the past.

By analyzing the chapter content of all nine volumes, as given in Table 2, although again with the caveat that this is a very small sample size, we can come to some more tentative conclusions.

Archaeological Chemistry Present

From Table 2, it is possible to discern a nearly clean break between the first seven volumes in the series and the last two volumes. There is an ongoing interest in artifacts comprised of ceramics, glass, pottery, metals and organic materials that falls sharply to zero after 2007. On the other hand, the final two volumes in the series expand into materials science, place greater emphasis on colorants and inks, and for the first time we see isotope analysis and dating the subject of three full chapters in volume VIII (although this was an ongoing subject in the previous volumes, but only peripherally). Thus, we might say that the 2013 and 2020 volumes represent Archaeological Chemistry as harbingers of the Present. Within the "present," we also see the history of archaeological chemistry and educational applications

Table 3. Subject Matter by Grouped Topics Addressed by Two International Symposia on Archaeometry (ISA) in 2016 and 2018 (inclusive of oral and poster papers)

Symposium	**41st: 2016 (13)**		**42nd: 2018 (14)**	
Subject Matter	**Number of papers**	**% (n=447)**	**Number of papers**	**% (n=268)**
Stone, Plaster and Pigments	102	21.8	68	25.9
Ceramics, Glazes, Glass and Vitreous Materials	127	27.4	63	22.9
Metals and Metallurgical Ceramics	102	22.2	59	21.9
Archaeochronometry	36	7.6	22	8.1
Human-Environment Interactions	53	13.2	42	15.5
Remote Sensing, Geophysical Prospection and Field Archaeology	21	5.1	14	5.7
From Bronze Age to Iron Age	6	2.7		–

addressed for the first time. At the same time, we recognize that the perceived break between Volumes VII and VIII represents a shift in the interests of the symposium participants and possibly an artifact of small sample size, but not necessarily a decline in interest in the traditional artifact groupings by the more universal archaeological community. Indeed, if we examine the subject matter addressed in Table 3 for two recent international symposia on archaeometry for which complete data were available, we get a more complete picture.

From Table 3, we can see that interest in all areas was quite similar with a slight rise in stone, plaster and pigments and a slight dip in ceramics. Almost all of them reflect the interests shown for the first seven of the HIST volumes with the exception of field archaeology and Bronze Age to Iron Age transition. This is to be expected given that archaeological chemistry and archaeometry are not exactly identical: archaeological chemistry is the subset of archaeometry in which chemical analytical methods are applied to the study of archaeological artifacts, not necessarily the entire battery of scientific measurement techniques. The important point is that the HIST volumes are not outliers in the general topics covered in these recent international symposia.

By breaking out the specific analytical techniques used in all nine volumes, we can come to an even greater insight regarding the perceived break noted in Table 2 moving into the 2010-2020 decade. Although 58 instrumental techniques were used in the nine volumes, those enumerated in Table 4 (n = 17) are those that were used more than twice.

It is easy to see that MS, FTIR, XRD and XRF continue to be the workhorses right up to 2020, whereas NAA, one of the principal methods used up until 2010, fell away. At the same time, methods not necessarily used, but very much discussed for the first time in the Armitage/Burton (2013) and Orna/Rasmussen (2020) volumes, are: counter immunoelectrophoresis (CIEP), enzyme-linked immunosorbant assay (ELISA), fiber optic reflectance spectroscopy (FORS), forensic photography, hyperspectral imaging spectroscopy (HIS), polymerase chain reaction (PCR), portable hand-held devices, radioimmunoassay (RIA), Raman spectroscopy, surface enhanced Raman spectroscopy (SERS), and short-wavelength infrared spectroscopy (SWIR). There are numerous other methods not even touched upon, but these seem to be the ones that may carry AC forward. However, our best insight into the present state of AC can be gleaned from the prefaces of the final two volumes, as given in Table 5.

Note that these two statements, the present state of affairs, have shifted the emphasis on instrumentation and artifacts to different considerations that had not been possible previously: *in situ* and non-destructive analyses using the appropriate equipment, new kinds of questions regarding space, chronology, materials and culture, and how to handle growing amounts of data in these areas. We would be remiss if we did not include the questions raised by the 12 papers in the special issue of *Accounts of Chemical Research*, 2002 (17): artifact methods of manufacture, material sources, degradation and conservation, and extraneous information to be derived from buried remains. The situation will shift again and, indeed, we can almost sense the seismic activity already underway among practicing archaeological chemists. The next section will query some of them with respect to what they see is the future of archaeological chemistry in

Table 4. Number of Times (>2) Specific Analytical Techniques Were Used in the 9 Volumes

Specific Analytical Techniques	**I: 1974**	**II: 1978**	**III: 1984**	**IV: 1989**	**V: 1995**	**VI: 2002**	**VII: 2007**	**VIII: 2013**	**IX: 2020**
Atomic absorption spectrometry (AAS)		2	5	1					1
C-14 dating		1	1	2	5	1			
Electron microprobe analysis (EMA)					2	2	2	1	1
Electron spin resonance (ESR)				1	2	1	1	1	
Elemental analysis (wet)		1	2		4				1
Fourier transform infrared (FTIR)			1	2	2	2	1	3	2
Mass spectroscopy (MS) and Gas chromatography mass spectroscopy (GC-MS)			1	2	5	2	1	7	3
Inductively coupled plasma-MS (ICP-MS)					2	1	8	1	1
Neutron activation analysis (NAA)	5	4	7	7	4	1	5		
Nuclear magnetic resonance (NMR)				1		1			1
Polarized light microscopy (PLM)			3		1	1	1	3	
Scanning electron microscopy (SEM-EDS)			2	3	1	1	2	5	
Stable isotope analysis	1	2		2	2	2	2	4	
Ultraviolet-Visible (UV-Vis) spectroscopy		1			1			1	1
X-ray diffraction (XRD)			2	1	2		2	3	6
X-ray fluorescence (XRF)		1	3	3	1	2	6	12	6

terms of methodology, treatment of archaeological sites, examination of archaeological artifacts, interdisciplinary interests, perspectives, evolutionary trends and cultural implications, to name a few (18).

As part of the present situation, Pollard observes that

> increasingly into the mid-20th century, we have been given a large set of legacy data, of varying quality archaeologically and chemically. This is something that current and future archaeological chemists need to come to terms with including the following options: (a) Ignore and use only "modern" data—this discards a large number of data, and is unlikely to be possible on any meaningful scale or (b) Adjust the nature of the question to the quality of the available data. I actually believe that some of the "legacy" datasets are the best quality analyses that we have, but obviously only for major and minor elements since the technology to measure trace elements came later. The large samples taken (inconceivable now) means that heterogeneity issues are minimized (unlike laser ablation techniques), and the self-checking of the analytical total is absolutely priceless—again, often not independently provided now.

Robert Tykot adds:

> There will always be limitations on the actual context of the artifacts analyzed (and many may not even have a context, but from surface or other finds), AND limitations on elemental analysis due to which elements were analyzed/reported and how the results are calibrated (and whether [they] can be directly compared with other studies).

Whither Archaeological Chemistry?

In 1996, and again in 2008, **A. Mark Pollard** and **Carl Heron** asked the question that is the title of this section (19). Where, indeed, did they see the science of archaeological chemistry going? First, in 1996, they

Table 5. Summaries of the Prefaces of Volumes VIII and IX of the Archaeological Chemistry Series (2013 and 2020)

Volume	Preface Summary
AC VIII: 2013 R. A. Armitage and J. H. Burton, Eds. (15)	AC "today is more than the usual studies of trace elements in pottery and lithics, which continue to contribute to our understanding of human behavior in the past. New areas of research include more focus on portability to analyze pigments *in situ* and artifacts in museums, nascent developments in non- and minimally destructive chemical characterization, new applications of isotopic analyses, and an increasing interest in archaeological biomolecules."
AC IX: 2020 M. V. Orna and S. C. Rasmussen, Eds. (16)	AC's "traditional fields of interest—matter, time, and place—have been transformed due to different kinds of questions about the past that modern methods of scientific examination are in a position to shed some light on. Enhanced capabilities, for the most part multidisciplinary in nature, have revealed the limitations of confining archaeological investigations to chronological, spatial, and material areas without also considering the cultural context, the power of combined analytical techniques, and the ability of chemometrics to handle large databases to help interpret results."

named a present reality: the availability of good quality, albeit expensive, analytical facilities. But laboratories are not the whole answer to the future of AC since they noted that emphasis would fall into the world of ideas, not practical matters. Good ideas come from good and relevant questions, from intelligent interpretation of results within a sound theoretical framework, leading, hopefully, to the better integration of archaeological chemical data. They also said that chemistry will have a very important role to play in materials conservation since it will be the chemists who will be best situated to understand the mechanisms of corrosion and strategies to mitigate its effects. Another future consideration would be the changing policies of the relevant local authorities with respect to handling the preservation of archaeological sites and artifacts, and the legal ramifications arising from such policies. For example, many countries have substituted policies of "preservation by burial" as opposed to excavation of archaeological sites.

In 2008, Pollard and Heron (20) continued their analysis by naming the three areas that have had the greatest impact on the archaeological sciences in the past 100 years: dating techniques, provenance studies, and studies in human diet, nutrition, status and mobility. They feel that these applications will steer the future direction of archaeological thinking. In addition, understanding material culture, but harmonized with other studies of social and cultural context of archaeological problems, promises to be a very useful area of investigation for the archaeological chemist. They frame the real restrictions to good AC in terms of the quality of thinking rather than practicalities, requiring careful construction of relevant archaeological questions and intelligent interpretation of results within a sound theoretical framework. Finally, as excavation sites are increasingly threatened by development, archaeological chemists will need to concentrate on studying deterioration mechanisms of archaeological materials and understanding of contextual variations leading to strategies for their control—a potentially political as well as scientific issue. They finish on a hopeful note: "the archaeological demand for qualified archaeological chemists or archaeologists with considerable chemical knowledge has never been greater."

Figure 1. *Bust of Queen Nefertiti excavated from Amarna. Treated as an archaeological object, the iconic headdress was found to have been painted with Egyptian Blue, calcium copper tetrasilicate. Public domain.*

Williams College archaeological chemist, **Anne Skinner**, asks a further relevant question regarding sites and burials: what about the existing controversy on whether to leave a portion of any site unexcavated, so that subsequent investigators can determine things not accessible now? Of course, she observes, this does not apply to the multitude of sites being excavated in advance of destruction, although there, perhaps, some samples could be archived.

Another important area of concern is the contemporary effort to broaden the number of people working in the field. Involvement of the local population and local archaeologists has been varied depending upon the perceived importance of archaeology to non-archaeologically attuned scientists in a given country. Skinner says that currently archaeologists (and many others), are being encouraged to involve people from the countries being studied, not just as laborers in the field but also as professional colleagues who lead projects. Many countries often do not have state-of-the-art facilities but the work being done is worth a hearing. She pointed out two *New York Times* articles that addressed these issues. One refers to efforts to "decolonize" archaeological field efforts by involving the local population from the beginning in terms of consultation, jobs, decision-making regarding the fate of artifacts and respect for the local culture (21). "Decolonization" also varies from country to country; presently, about half a dozen South American countries are carrying out their own scholarly work in excavations and artifact analyses, and many countries limit the removal of artifacts from their territories. The other *NYT* article addresses a similar question but delves more deeply into problems like squabbling over turf, overstretching conclusions from minimal data points, and the danger of "imperializing" archaeology. Specifically, the issue is the continuing improvement in instrumentation and methodology to allow more precise analyses, perhaps on smaller samples and new materials. This very fact will continue a move towards centralization of labs since these new instruments are not cheap, either to purchase or to run, leading to significant fees for users. In some cases, they require great skill in order to obtain optimum results. However, these centralized labs then may end up controlling what work is done. Only those who can afford the charges and whose work interests the operators will have access. More seriously, those who cannot use these high-quality labs may find that they are unable to publish their work (except, of course, in predatory journals), because reviewers will ask to see the "better" data. An example of the perfect being an enemy of the good, as they say (22).

Another issue regarding "decolonization" was the established pattern beginning in the 18th century for European scientists to transport their colonies' natural treasures to deposit them in museums in their home countries. An example is shown in Figure 1. In 1912, the exquisitely painted limestone bust of Nefertiti was excavated at Tell el-Amarna and promptly packed off to the Staatliche Museen zu Berlin. "Legal" or not, Nefertiti became the focus of a growing national outrage at what was perceived as foreign exploitation and appropriation of Egyptian heritage (23). There are many equally famous examples of what many now regard as plunder permanently ensconced in museums far from their origin. The Rosetta stone and the Parthenon sculptures come immediately to mind—with all of the legal ramifications attached thereto. What if the home countries demanded restitution of these artifacts and how would the possessors respond? We already know some of these answers. There may be many more issues to address in the future.

I have direct experience of an event that took place in Israel that addressed this problem front and center. Following the June 1967 so-called six-day war between Israel and its three adversaries, Jordan, Syria and Egypt, Israel's archaeologists moved into its vast newly occupied territory in the Sinai and began a major excavation program that ended in 1982 when the Sinai was returned to Egypt. They investigated over 1300 hitherto untouched archaeological sites that lay beneath the sands and unearthed thousands of artifacts including pottery sherds, jewelry and tombstones. Cataloguing, dating and analyzing this trove took decades and was still not complete by December 28, 1994, which is where I come into the picture. I spent a Fulbright year in Israel (1994-1995) and was invited to the December event, a reception at the Rockefeller Archaeological Museum in Jerusalem, to honor the Egyptian archaeologists who had come to receive back their artifacts as a condition of the peace treaty between Israel and Egypt.(24, 25). Although it took two more years to effect the transfer, under the terms of the treaty, it took quite a few more years for the artifacts to find disparate homes in Egypt. One of these sites was at Al-Arish, about 30 miles west of the Egypt-Israel border where a national museum was built in 2008 to, admittedly, simply "warehouse" the artifacts (26). The second is the Museum of Taba City on Pharaoh's Island where over 700 of the Sinai artifacts are on display and are touted as a major tourist destination (27, 28).

University of South Florida archaeological scientist **Robert H. Tykot** weighs in on the major technological advances and changes in the practice of archaeological material studies that have taken place in this millennium.

> Separate from advances in the study of ancient DNA, stable isotope analysis, proteomics, and drones used for 3D mapping, light detection and ranging (LiDAR), NIR, and other remote sensing, I see the ability to conduct non-destructive elemental analysis using hand-held portable X-ray fluorescence spectrometers (pXRF) as having the greatest archaeological chemistry impact on archaeology. It has specifically enabled analysis of objects within museums and storage facilities around the world, saving destructive sampling, transport, and international permission, while providing rapid and low-cost yet quantitative analysis of major and trace elements. Starting in 2007, I personally have used this on more than 10,000 obsidian artifacts from 300 sites throughout Italy, allowing statistical comparisons between sites and time periods (29). I have also used pXRF on objects that could never be destructively sampled, including museum display metal artifacts (e.g. copper alloys, silver/gold alloys), ceramics, cave paintings (in situ!), and other cases (30). The "educated user" can properly calibrate the results, and deal with surface analysis interpretations, just as with regular XRF and SEM-EDS users have done in the past. While even the latest pXRF models (I have the Bruker 5g) are not a substitute for regular XRF, or ICP-MS or INAA instruments (all producing results for more elements), which either require powder samples or a small object to fit in the machine, the ability to take samples for analysis outside of museums and especially from foreign countries has decreased significantly. This is a result of political and institutionalized management of museum and other past collections, the increased importance of conservation on museum collections (see the unfortunate event of the major national museum fire in Brazil in 2018 (31)), and the scientific limitations of non-destructive pXRF poorly understood by non-scientist museum officials. Nevertheless, I expect the development and use of pXRF and other non-destructive analytical instruments to increase even more in the future.

Another area of study that has expanded considerably in the past several decades is stable isotope analysis of human remains as a means of studying ancient diets, explains Tykot. In his recently published encyclopedia article (32), he outlines the principles, methodology, data that can be obtained, and future directions for this approach. Some of the chief issues currently being addressed are early hominin dietary practices, Mesolithic-Neolithic dietary changes, migration and mobility, dietary practices based on gender or on social status, and the importance of staple foodstuffs like maize and millet in different populations. Future directions will include expanding the number of elements used to study diet and methods to decrease even further the sample size necessary for analysis.

Following up on Rob Tykot's analysis, Professor **Ian C. Freestone** of University College London Institute of Archaeology makes four important points:

- "Synchrotron techniques need to be used more constructively to address real problems. For example, we have used X-ray absorption spectroscopy (XAS) to determine oxidation states of Fe, Mn and so on but the results should be calibrated against replica compositions run in gas-mixing furnaces to determine… conditions of firing" and ultimately, quantitative phase compositions of ceramic bodies and glazes.
- "The identification of small production groups or production events can enable an understanding of production organisation (e.g., The work of Martinón-Torres on the weapons of the Terracotta Army (33)) and the recognition of sets and consignments so we can understand how artefacts were procured (e.g., work we have done on glass)."
- "While we are aware that metals and glass were recycled it is challenging to determine the relative intensity of the recycling process…[so it might be] possible to come up with some qualitative indicators… [of] assemblages and societies." (34)
- "On the instrumentation front, we need development of portable laser micro-sampling of artefacts as a routine approach so it can be used in the field and samples taken back to the lab for isotopic and elemental analysis."

Zvi Koren, Director of the Edelstein Center for the Analysis of Ancient Textiles and Related Artifacts at Shenkar College, Israel, muses on the role of color in AC, among other things:

> What I would like to see in the future of archaeological science and conservation are approaches that would be truly interdisciplinary. Of course there are the "regular" ideas such as developing and improving non-destructive testing (NDT) of various pigments, dyes, and other non-colorant residues (food, drinks, cosmetics, etc.) What truly fascinated me about 15 years ago when I first saw it in the Istanbul Archaeological Museum was a colorful recreation of a tall statue of a Greek or Roman woman… This was a colored image of what the statue may have looked like when it was first created according to the artist that rendered this image.

(Author's Note: The statue was the Peplos Kore as Artemis reproduction of an original from the Athens Acropolis that is part of a traveling exhibit called "Gods in Color" from the Munich Glyptothek. Figure 2.)

***Figure 2**. Peplos Kore as Artemis (ca. 530 BCE) Polychrome Restoration. Wikimedia Commons (https://commons.wikimedia.org/wiki/File:NAMABG-Peplos_Kore_as_Artemis.JPG).*

> The big picture is this: For quite a while now, archaeologists, museum curators, conservators, and scientists realize that many of the Greek and Roman and much older statues that today have a practically white and colorless appearance when quickly looking at them, were originally colored/painted. A close inspection of some of these statues, even with the naked eye, one could still see residual pigments. Obviously with some magnification more colors may become apparent. Hence, the scientists would scan the object with a non-destructive technique, such as XRF, in order to identify these pigments, and also, if needed, micro-sampled in a minimal invasive method, then the pigments would be identifiable. Now the conservation artist can take over and propose an image of how the statue first appeared. This image (of course not needed to be the full size of the statue) would be placed next to the statue to get a "wow" moment of the grandeur of that artistic work.
>
> In my museum visits I often go right up to the object, if allowed, and visually look for these "nearly invisible" colorations and have seen them on various pieces, including Assyrian sandals on the long stone reliefs in the British Museum. These are not quite 3,000 years old and amazing to see. I would love it if these would be studied, and offer an artistic rendition of what they looked like. Many other such cases exist.
>
> But not only statues, of course, but structures, buildings too. For example, during a family hike, we came to an ancient synagogue (possibly about the 5th century CE) in *Ein Keshatot* ("Spring of Arches") in the Golan. There was an earthquake in this area so that all the stones of the synagogue came tumbling down and since there were no major villages nearby, practically all the synagogue's stones were still present at this site (and not carried away for secondary usage). This synagogue was excavated and reconstructed with advanced technological methods by scanning each brick and digitally putting the stones together as one giant 3D puzzle. (That is another interesting method for future archaeological conservation and preservation.) But my main point is when I inspected the reconstructed Holy Ark, on its columns you could still see residual blue rings at the top and bottom that decorated the 2 columns. I haven't seen that reported on and like many other sites, it would be wonderful to analyze that and the rest of the Ark's structure.

Scientific Director of the Biomolecular Archaeology Project at the Penn Museum, **Patrick McGovern**, summarizes much of what has already been said with a global spin on a science that has evolved in mini-steps with its eyes literally on the ground (and underneath it) to capture and then analyze artifacts:

> Archaeological Chemistry or Biomolecular Archaeology is the "wave of the future" in archaeology. By rigorously applying ever more precise chemical and archaeological techniques, this nascent, highly multidisciplinary field, blending together the humanities and sciences, holds out the prospect of uncovering much more of what it means to be human biologically, medically, and culturally over the past 4 million years and more. Optimistically, we might envision a "new history of humankind" eventually being written. This prospect was adumbrated in this writer's 1995 "Science in Archaeology" piece (35) and, most recently, in the updated Afterword to his *Ancient Wine: The Search for the Origins of Viniculture* (36). Ancient viniculture exemplifies how Archaeological Chemistry can be integrated into a holistic investigation of a truly remarkable plant and its product intertwining itself with human culture and technology around the world."

Joseph B. Lambert, archaeological chemist at Trinity University in San Antonio, is concerned for the professional future of AC in the United States. He says that here,

> future directions for archaeological chemistry largely will follow the money. The field is well funded and active in Europe, especially England, and Asia, but there is no stable, major, external funding in the United States. Consequently, the field tends to be an avocation for individuals at major universities or a focus for individuals at liberal arts colleges and other places where outside funding is not the driving force. The most successful models in the United States are museum laboratories and archaeology programs. Both venues have long invested in archaeological technology (dating, prospection, and elemental/molecular analysis). The Getty and the Smithsonian have excellent programs, and other museums also are very productive. Noreen Tuross is Landon T. Clay Professor of Scientific Archaeology at Harvard, and Nikolaas van der Merwe preceded her in a similar position there. Douglas Price, now retired, established the Laboratory for Archaeological Chemistry at the University of Wisconsin Madison and was elected to the National Academy of Sciences for his archaeology and archaeological chemistry in 2018. They attracted strong funding for archaeological chemistry and carried out significant research in the field over a long period of time. All three are primarily archaeologists rather than chemists and represent the model that will be most successful in the future for making broad contributions to the field.

Similarly, Heather Lechtman at MIT has been a major influence in the development of archaeology and archaeological chemistry for over half a century. The Center for Materials Research in Archaeology and Ethnology, established by Lechtman in the late 1970s, has produced a large cadre of science-oriented archaeology faculty.

Mark Pollard, having raised the question of "whither," gets the penultimate word:

> [L]ooking forward, some things are obvious. The big change over my career is that when we started we often had to build the equipment ourselves—I started at York and Oxford by building an XRF system, and writing a computer programme (in Fortran!) to carry out the necessary primary and secondary absorption corrections. We are now, for better or worse, largely in the hands of the instrument manufacturers—very few innovations are made specifically for archaeological/cultural heritage purposes—perhaps the last was the combined XRF/XRD for pigment analysis on paintings and manuscripts.
>
> This is good and bad. It is good because we have available an amazing range of analytical and isotopic tools—many are too expensive for archaeological labs to purchase, but usually access can be arranged. The downside is that they have become black boxes—not just pXRF, but, for most instruments now, it is very difficult to find out what the processing software is actually doing. This is not necessarily a problem providing that great care is taken with primary and secondary standards, but this is rarely done, and even more rarely reported. The explosion of pXRF is a particular issue—it has "democritised" analysis, but can produce unhelpful results. The key question for me is what is the analysis done for—is it to answer a specific question (e.g., is this coin gold or electrum, etc.), or is it intended to produce an analysis of record, which can be used by others? pXRF is probably best suited to the former in most cases.
>
> There are now methods of analysis available archaeologically which were undreamt of in the 1970s. Examples especially are in the field of organics—compound specific isotopic methods, proteomics, etc. These open up new fields of research—I am particularly interested in the potential for copper corrosion products to retain organic evidence from vessel use—which requires some knowledge about organometallic chemistry.
>
> Another good thing is that archaeology now has a good number of trained chemists working within it. When I started, the model for "archaeometry," at least as expressed by Martin Aitken (1922-2017) (37), was to get a "trained scientist" and a "trained archaeologist" to work together. This distinction has largely gone in archaeology, with some trained scientists working *within archaeology*—I think this is important, because, with the best will in the world, we have seen too many specialisms arise in science departments as a result of individual enthusiasm, only to disappear on retirement. There is always a place for specialised collaboration, but I think mainstreaming chemistry into archaeology, at least to the level of "informed consumer" has been a good achievement—albeit with the potential for people stepping outside their competences occasionally!
>
> I have a bit of a bee in my bonnet about the distinction between archaeological science and heritage science. Both focus on the examination of artefacts (ranging from trace deposits to landscapes), but the intentions are quite different. At least in my definition, archaeology is about people—the analysis of objects is a stepping stone to understanding the activities and intentions of people in the past. Heritage science is about objects—it includes manufacturing techniques, but also includes conservation, restoration, presentation, etc.
>
> For me, the measure of success in archaeological chemistry is the extent to which the work changes the archaeological narrative—a good example would be the earlier appearance of milk in the archaeological

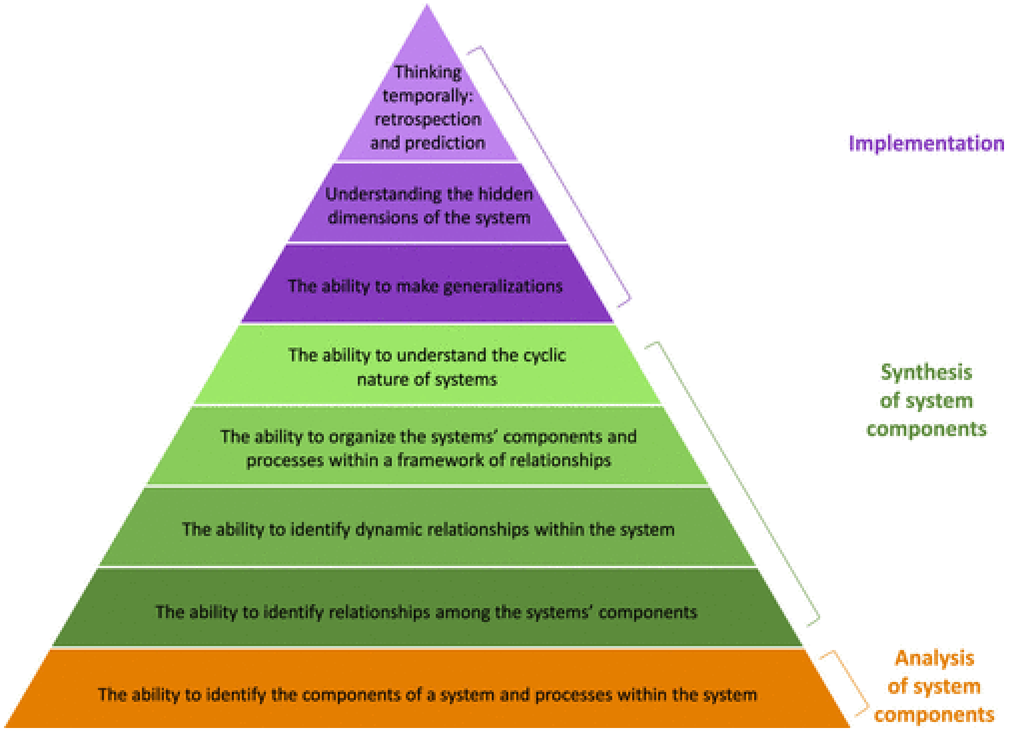

Figure 3. *Systems Thinking Hierarchical Model Pyramid from Ref. 40, https://pubs.acs.org/doi/10.1021/acs.jchemed.9b00169. Used with permission. Copyright 2019, American Chemical Society. Further permission related to the material excerpted should be directed to the ACS.*

> record than had otherwise been expected, but there are many others. I think I am more interested in the quality of the question than the sophistication of the chemistry applied, although it is clear that novel chemistry can allow old questions to be revisited, or new questions to be addressed.

Conclusion

As the author of this essay, I reserve for myself the last word. Throughout the speculative and hope-filled contributions of the distinguished archaeological scientists whom I queried, our eyes were lifted to the heavens to visualize a future that transcends material objects in order to include meaning, culture and context. This future is, in fact, inevitable given the greater complexity of techniques that drives the formerly simple questions of "what," "when," and "where" into areas like human modes of operation, environmental conditions, and other concerns. These factors have shifted chronological, spatial and material limitations to another level. For example, in addressing the question of time, the archaeologist turned novelist Karin Altenberg remarks, "The exploration of the past is an exercise in empathy, a way of becoming conscious of what it is to be human in another time and place" (38). There was a time when archaeology was all about finds, i.e., artifacts that had shouldered their way into the present. Now it is all about the absence that emerges from our examination of the artifact: what are the blanks that have to be filled in? Is the instrumental arsenal at hand enough, or do we need additional tools and information? Pollard hinted at how the existence of some of this information in the form of legacy databases could help. Are we finding ways and means of writing a new history of humankind, as conjectured by Pat McGovern? What happens to our science when we begin to be all-inclusive, as examined by Anne Skinner? Does broadening out lead to dilution or to enrichment? Any archaeological object is like a two-sided coin: a part that has passed and a part that remains. The part that remains can be queried about its role in the past. The part that has passed remains shrouded in mystery unless, bit by bit, the context for its fabrication and use can be pieced together from external evidence (39).

All of these questions cry out for a paradigm shift in our practice of the discipline. We are being called to reverse our gaze, to zoom out from the discipline-bound outlook of the past to embrace a more holistic view of archaeological chemistry and its intimate connection with a network of societal systems. The entire issue of the

Journal of Chemical Education for December 2019 was devoted to examining this possible U-turn (view-turn) with respect to chemical education. Such thinking invites us (a) to visualize the interconnections and relationships among the parts of a system, (b) to examine how behaviors and attitudes change over time and (c) to examine how systems-level phenomena emerge from interactions among the systems' parts (40). Acknowledging that archaeological chemistry is inherently multidisciplinary has not helped much in moving us completely out of our individual silos. A helpful graphic representing an analysis, synthesis and implementation of system components that are common to virtually every discipline (Figure 3) might enable us to discern where we are on the pyramid.

Making us aware of and appreciating the continuous presence of the past in our lives is a work-in-progress of the archaeological chemistry community. Becoming more aware of the global nature of that presence may be a way forward toward realizing that more complete and inclusive new history of humankind that we all desire.

Acknowledgments

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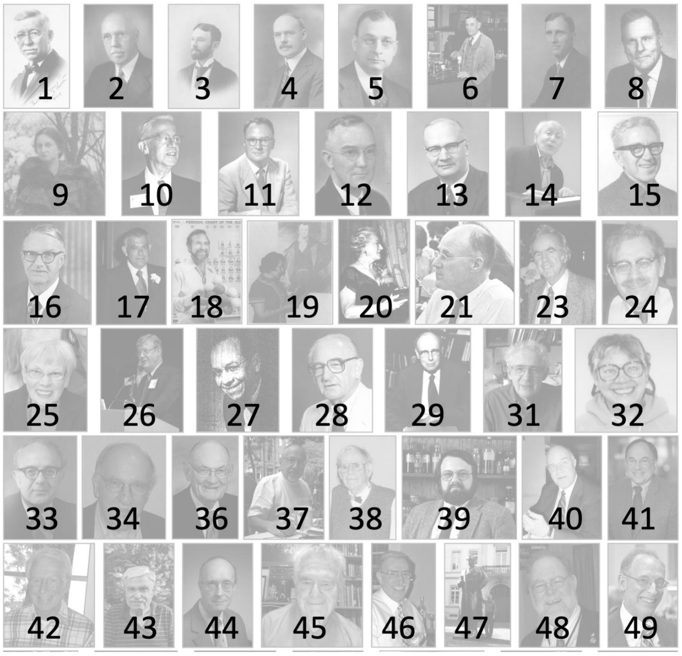

Chairs of HIST: Key to the Cover

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2	Charles A. Browne	1922-23
3	Frank B. Dains	1923-26, 1933-34
4	Lyman Newell	1927-32
5	Tenney L. Davis	1935-39
6	James Couch	1940, 1941
7	Harrison Hale	1942-46
8	Henry M. Leicester	1947, 1948-51
9	Virginia Bartow	1952-54
10	Eduard Farber	1955-56
11	Wyndham D. Miles	1957-59, 1965
12	Virgil R. Payne	1960-61
13	Aaron J. Ihde	1962-64
14	O. Theodor Benfey	1966
15	Martin Levey	1967
16	Melville Gorman	1968
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42	Paul R. Jones	1994
43	Martin D. Saltzman	1995
44	Joseph B. Lambert	1996
45	Harold Goldwhite	1997-98
46	Stephen J. Weininger	1999-2000
47	Richard E. Rice	2001-02
48	David E. Lewis	2003-04
49	Jeffrey I. Seeman	2005-06
50	Roger A. Egolf	2007-08
51	Jan Hayes	2009-10
52	E. Thomas Strom	2011-12
53	Gary D. Patterson	2015-16
54	Ronald Brashear	2017-18
55	Daniel Rabinovich	2019-20
56	Seth Rasmussen	2021-22

CAN WE BRING CHEMISTRY BACK? EXPLORING THE POTENTIAL OF "GATEWAY ARTIFACTS" AT THE SCIENCE HISTORY INSTITUTE

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Abstract

For decades, science museums in Europe and America have been reducing the exhibition space they allocate to the presentation of historical chemical artifacts. This paper discusses several factors behind this concerning phenomenon, including changes to science museum revenue models, shifts in those museums' target audience profiles and interests, and the lack of aesthetic appeal exhibited by many chemical artifacts. It argues that the relative absence of these artifacts in museum displays deprives audiences of opportunities for unique, non-text-based learning experiences in settings that are especially conducive to engaging with material culture. The paper concludes by advocating for the design of single object "gateway artifact" exhibits that encourage museum visitors to examine and interrogate chemical artifacts from multiple perspectives; such exhibits could catalyze audience interest in the history of chemistry and provide museum visitors with critical tools for "unpacking" the scientific artifacts they encounter in museums and in their daily lives.

In 2025, Tsinghua University in Beijing will unveil its new "Tsinghua Science Museum," an institution whose projected size (it is planned to exceed 30,000 square meters) and programmatic ambitions will immediately place it in the upper echelon of university science museums worldwide. Informed by the leadership of Tsinghua's burgeoning Department of the History of Science, the Tsinghua Science Museum is being designed, in part, around a mandate to serve public audiences, with a focus on school-age children. Consequently, it will feature exhibitions on themes in contemporary science and innovation, driven by the latest in interactive exhibit technologies. Consistent with the aims of the historians of science who are guiding its development, however, the museum will also earmark considerable space for the presentation of artifacts drawn from the histories of Chinese, European, and American science.

With curation of their museum's future chemistry galleries in mind, Tsinghua's history of science faculty plan to build a core collection in this discipline; in their proposed long-rotation exhibition scheme, even artifacts that curators recognize could be intellectually stimulating but perhaps "visually disappointing"—the twentieth-century instruments or proverbial "black boxes" that challenge audiences with their inscrutability and modest aesthetic appeal—will be prominently featured. To this end, they have expressed interest in securing long-term loans of chemical apparatus and twentieth century analytical instruments from the Science History Institute's permanent collections. The Institute will be delighted to comply with this request for loans and for participation in collaborative projects with Tsinghua, encouraged in part by the realization that a major new museum is committed to borrowing, exhibiting, and programming around the types of historical chemical artifacts that, ironically and for many decades, have been gradually *disappearing* from exhibition halls in peer science museums in Europe and the United States.

This disquieting phenomenon has been well-chronicled by scholars in the history of science and museum studies, who have also commented on a parallel trend: the rapid global growth of science centers, whose exhibits and programming typically rely on interactives to engage their target youth audiences. Interactive-intensive exhibition tactics can, to be sure, support effective, constructivist pedagogical approaches to introducing people to abstract scientific concepts and practices, particularly as those concepts are embedded in contemporary environments and technologies. These approaches, however, have too often been pursued, wittingly or not, at the expense of presentations—and stories—that rely on historical artifacts to engage audiences.

Robert Anderson called attention to this development in his provocative 2016 Bunge Prize lecture, "Where Has All the Chemistry Gone?" (1). Anderson's question invites reflection (on why a shrinking population of small private museums and university collections, rather than large, nationally funded institutions, have become the last redoubts of historical chemical artifacts) as well as responses: what can we do to ensure that chemistry's material heritage is increasingly made visible and deployed to generate audience interest, questions, and perspectives rooted in the *history* of this discipline? If Tsinghua University's positive commitment to providing a museum platform for the history of chemistry is not to be anomalous, and if we are to "bring back" the chemistry that has been leaving our exhibition schemes, we must reckon with some of the reasons why chemistry's historical artifacts no longer have firm footing in today's museums.

Going, Going…Gone?

A steady decline in exhibition space devoted to historical artifacts in modern science museums over the course of the twentieth century has been well documented (2). Major, publicly accessible science and technology museums that made significant commitments to artifact presentation in the late nineteenth and early twentieth centuries (such as the Deutsches Museum, the Science Museum, London, and the Smithsonian Institution) did so primarily in the interest of educating audiences employed in, or inclined to pursue, careers in scientific and technical fields. This agenda complemented another, traceable in part to the influence of the international expositions and trade shows of the age: to use museums or museum-like displays to stimulate appetites for, and develop perspectives and skills that would further, scientific and technological innovation, and thus contribute to economic progress. Display schemes during this period tended to feature the presentation of massed collections of historical artifacts, chemical and otherwise, in large glass cases in what today might be referred to as "open storage" arrangements. Historical and contemporary objects were typically blended, and object labels tended to focus on the scientific principles and technical operations manifested in the apparatus and instruments, and on their utility, rather than on constructing narratives through which audiences might have viewed artifacts as emblematic of significant historical trends and developments.

As a case in point, Peter Morris's recounting of the evolution of exhibition schemes in the chemistry galleries at the Science Museum, London, through the twentieth century describes a development trajectory similar to those presented by several other science museums in Europe and the Unites States during this period (3). Morris describes the Science Museum's increasing interest, beginning mainly in the 1920s, in portraying the *history* of chemistry through artifacts; this approach culminated in the Museum's 1977 redisplay of more than 11,000 square feet of chemistry galleries. In these historically focused displays (complemented by nearby galleries devoted to the chemical industry and the public benefits it generated), chemistry was treated as a science with a history traceable to the ancient Egyptians, encompassing important contributions and related artifacts from the medieval and early modern periods and culminating with an illustration of major chemical developments of the twentieth century (4).

The Science Museum's 1977 chemistry galleries presented the visiting public with narratives of historical continuity, articulating how chemistry's past academic and research achievements had been instrumental to the development of useful industrial applications over time. These narratives were supported by and designed around the strategic acquisition and display of significant historical objects (particularly twentieth century instrumentation) by curator Anderson. In place for more than twenty years, the 1977 installation represented the apogee of the Science Museum's commitment to presenting the evolution of chemistry through historical artifacts. In 1999, however, these exhibitions and their artifacts were de-installed in favor of a new presentation, "The Chemistry of Everyday Life," which occupied only 13% of the original 1977 spaces devoted to the history of chemistry. This exhibition relied on a new suite of exhibits to focus on themes such as the development of chemistry since ~1800 (emphasizing quality control and biochemistry), contrasts between pure and applied chemistry, and the presence of chemistry in contemporary life in unexpected places. The earlier focus on original artifacts as vehicles for carrying historical narratives yielded to a new reliance (at least initially) on interactive exhibits.

The interpretive arc traced by the development of the chemistry presentations at the Science Museum, London, was also in evidence at other peer science museums, such as the Museum Boerhaave and the Museum of Science, Boston, during the late twentieth century (5). As Anderson noted in his Bunge lecture, the world's major science museums have almost completely abandoned artifact-grounded presentations of the history of chemistry (and of the histories of other scientific disciplines as well), while the science centers that have been founded over the past fifty years primarily deploy interactive exhibits to illuminate STEM concepts, and the useful contemporary applications built upon them, with scant attention to the historical antecedents of those achievements. For chemistry, the task of preserving and interpreting the field's material heritage has largely fallen to a relative handful of small, specialized museums and university-based collections, which typically attract neither the resources nor the public attention necessary to meaningfully leverage historical collections for audience engagement.

Why Has the History of Chemistry "Left" Our Museums?

So, it appears that the history of chemistry has indeed been "leaving" our largest science museums—but why? Financial pressures have certainly played a role: state-sponsored institutions (particularly those in Europe and Asia) rely on governments for the bulk of their operating funds and government funders expect a return in the form of robust public attendance figures. The sobering fact is that museums dedicated solely or primarily to presentations on the history of chemistry typically draw very small audiences (6). In the United States, where government funding normally comprises only a small portion of operating budgets, philanthropy must make up the difference and philanthropy usually follows the turnstile. Museums and science centers believe that interactive-heavy exhibitions on recognizable themes are popular with their target audiences of children and their care givers, and attendance statistics and financial performance bear this out (7).

These financial realities are, of course, not just cause but also an effect of changes in audience composition and behavior. Science museums and centers have, for many decades, been gradually aiming their holdings and programs at non-expert audiences and have only recently focused on gathering data on the interests of the public (8). As Andrew Nahum observes, the increasing lack of sophistication in target audiences for science museums can be mapped onto a parallel shift in presentation tactics, from the earlier display of "study collections" of scientific artifacts (whose purposes and functions would have been apparent to scientists and practitioners) characteristic of galleries in the late nineteenth and early twentieth centuries, to the design of "games of communication" in recent decades, in which visitors need to be interactively entertained, as well as informed, to keep them coming in numbers (9).

Compounding the challenge of engaging scientifically unsophisticated audiences is the relative lack of superficial aesthetic appeal exhibited by chemistry's historical artifacts; chemistry, as numerous commentators have observed, lacks what Ad Maas refers to as "showpieces," or objects with "remarkable appearances" that have the "charisma" to attract viewers' attention, especially in the absence of familiarity with the objects' uses and purposes or sufficient contextualizing historical information (10). This is especially true of so much twentieth century instrumentation, for which the wryly ascribed term "black box" is often apt. Audiences not immediately familiar with the inner workings of these technologies are often bemused by their unadorned, sleek, modernist designs and the lack of surface indices of internal operations or instrumental uses. And these machines, often resistant to visual engagement and interpretation, are also tangible reminders of the relative inscrutability of modern chemistry itself, whose objects of research are complex and, unlike many of their counterparts in physics and biology, difficult to actually *see* or imagine.

This problem with visualizing the nature of chemistry itself is compounded by the fact that chemistry's physical manifestations in our lives and impacts on our behavior, while ubiquitous, are usually embedded in such a way that the presence of chemical phenomena all around us is not obvious. On this paradox, Ruth Jarman has observed that: "while chemistry makes an immense contribution to almost every aspect of modern living, a number of research studies have reported that many young people and adults fail to recognize its relevance to their daily lives" (11). Chemistry—its present and past—is literally and figuratively "hidden in plain sight."

The difficulty the public experiences in recognizing chemistry in daily life, let alone evidence of the history of chemistry, translates into challenges in the classroom and in museums. In recent years, educators and museum professionals have consistently experienced resistance to well-intentioned schemes to introduce content on chemistry and its history into learning and cultural environments. At the heart of this public resistance to engagement with chemistry lies a perception that the field, along with being obscure and synonymous with abstraction and mathematical puzzles, is also partly responsible for many environmentally and socially harmful practices. Zaragozo and Fernandez-Novell remark on this phenomenon as they have observed it in Spanish secondary schools; they argue that misperceptions about the roles that chemistry plays in our lives and ignorance of the nuances of that interplay are, ironically, connected to the absence of history of chemistry content in courses, in museums, and in the mass media (12). Chemistry, in multiple respects, has an "image problem."

To be sure, historical artifacts can "earn" places in museum displays through more than just their accessible and charismatic appearances; they can also appeal to visitors by serving as what Ad Maas has called "key pieces" or reference points in compelling storylines about the histories of their fields (13). When the historiography of chemistry was focused primarily on chronological narratives of the field's "heroic" investigators and innovators and their notable achievements in the laboratory and in the public sphere, it was a relatively simple matter for museum curators to connect those major principals to iconic artifacts that gave tangible testimony to their accomplishments. This approach had, and still has, strong appeal for visitors and thus to museums concerned with selling tickets.

In recent decades, however, new historical methods and perspectives have emerged in academe that have both challenged and enriched traditional historiographical approaches in the history of science—and caused museum curators to take notice (14). Along with traditional figures and sites of investigation (such as professional scientists and laboratories), new actors and spaces (technicians and artisans, hospitals, factories, and domestic settings) have been introduced as objects of research, contributing to a multiplication of novel research sources and methods (15). This expansion of the scope of historiographical approaches to chemistry has also opened what is perceived as a philosophical "fault line" between historians: scholars and practitioners on one side of this divide are viewed as concentrating primarily on those questions, theories, practices, and knowledge products deemed "internal" to chemistry as an academic scientific discipline, those on the other side as engaging in research that focuses on understanding chemistry in the context of social and cultural discourses. Sensitive to this dynamic, many museum curators have begun to question the centrality of iconic historical artifacts to exhibition narratives, often producing exhibitions in which historical objects have their presence reduced or obviated altogether—and history of chemistry exhibitions have been no exception to this trend (16).

When the History of Chemistry Leaves Museums, What Do We Lose?

As chemistry's historical artifacts have gradually "gone missing" in contemporary museums and science centers, what have been the consequences for audiences with learning goals—and for curators keen to address their interests?

As Hasok Chang has recently observed, chemistry itself is very much about "making;" Berthelot once famously said that "chemistry creates its object." Few scientific fields can match chemistry in offering historical examples where practical applications, often driven by industrial and consumer demand, have yielded useful products that, in turn, have generated future questions for inquiry and subjects for investigation. And these products have been made available to the broad public through wide commercialization in fields such as pharmacology and nutrition and through a vast range of manufactured goods—artifacts that can be made accessible as learning tools to audiences through museum displays in ways that theories, equations, and small molecules cannot (17).

In-person, vivid encounters with artifacts in museums, and the generation of historical insights and knowledge creation that they can support, cannot be easily replicated by reading texts. Advocates for integrating material culture studies into the history of chemistry, such as scholars who have undertaken to re-create past experiments and historical laboratory conditions and processes, point out that "sensual experience can be difficult to transmit textually" and that "the sensual experiences of reproducing an experiment can thus offer the historian otherwise unobtainable hints regarding the origins of ideas, theories, conclusions, or the subsequent pathways of investigation followed by historical actors" (18). Thinking in a similar vein, Chang captures succinctly the potential for the history of chemistry to be presented in ways that appeal to a broad spectrum of audiences: "the sensory world of the chemist is luxuriously multi-modal" (19).

Education theorists have observed that non-traditional spaces for learning (i.e., sites outside conventional classrooms, lecture halls, or the covers of textbooks), that are well-suited to engaging audiences with the material culture of the history of chemistry, can make ideal venues for enacting object- and experience-rich "multi-modal" learning. Museums, for example, can offer visitors spaces to move around objects, the occasional integration of multi-sensory stimuli (engaging sounds, smells, and other changes in ambient environment), access to library materials that complement object-based experiences in the gallery, and even (increasingly) chances to handle and examine artifacts from multiple perspectives. The remaining, and relatively few, global institutions that collect, preserve, and program around the rare books, works of art, archival materials, apparatus, instruments, and realia of the history of chemistry can be ideal places for enacting multi-modal learning for curious audiences.

Bringing Chemistry Back: Exploring the Potential of "Gateway Artifact" Exhibits

Given the capacity constraints—financial, human, spatial, and technological—faced by the small museums and university collections that still harbor and program around historical chemical artifacts, how might we develop strategies for the curation and continued presentation of such artifacts that are viable and deliver audience impact? This is a question faced by the Science History Institute, which, alongside its substantial and important library and archival collections, operates a museum dedicated to chemical history, with particular emphasis on nineteenth and twentieth century stories of chemistry's industrial applications and instrumentation. Through this museum, the Institute remains committed to the active collection and preservation of chemical artifacts, both for the benefit of current researchers and audiences, as well as of those in generations to come.

The Institute's museum also supports, and periodically refreshes, a permanent collection presentation, *Making Modernity*, originally curated in 2008. This exhibition features a visually compelling design and strikes an audience-friendly balance between artifacts, graphics and text. And yet, despite intelligent and creative efforts on the part of curators to connect with walk-in, lay visitors (as well as chemists and industry practitioners, the primary audience targets for the original design), this permanent exhibition faces many of the aforementioned challenges in its quest to engage the scientifically curious but largely uninformed public (20).

To address these challenges, museums like the Institute's should consider their strengths and limitations, not purely in a vacuum, but sensible of the resources and programming offered by the cultural institutions in their "peer ecosystem." Curators-cum-storytellers at small institutions can be excused for succumbing to the desire to present artifact-packed, ostensibly "comprehensive" exhibitions, but this impulse should be curbed in favor of exploring content niches and narrative approaches not already well covered by peers, as well as by adopting a "less is more" approach to narrative scope and numbers of objects presented. Moreover, like its peers, the Institute should be sensitive to the need to respect "sunk" investments in existing exhibition infrastructure; the immense expense associated with overhauling permanent exhibitions when interpretive fashions change places a premium on taking a different approach—generating cost-effective, innovative tactics for engaging, enlightening, and entertaining audiences that complement, rather than necessarily replace, the permanent exhibition status quo.

This stance urges on small but chemistry-rich museums the imperative of operating more like the historical laboratories they often describe and interpret, embracing a spirit of experimentation in their curatorial work. For museums open to curatorial experimentation, scaling audience impact will likely be achieved not solely through engaging the visitors coming through their own doors, but rather through the introduction of interpretive models that other peer institutions may be inclined to emulate and scale further.

With these parameters in mind, the Science History Institute museum will embark on a modest experiment in engaging its core audience (members of the public over twelve) in an exercise in interpretive skills building. Our proposed project will be the construction of a permanent, single-artifact exhibit, to be positioned in the museum's entrance hall, where it will be encountered and engaged by all Institute patrons; it will, in this setting, serve as their introductory, framing experience of the Institute. Every object that serves as the subject of this exhibit will be drawn from the museum's chemical artifacts collections; choices will range from the charismatic and prepossessing (Eighteenth-century brass balances? Early modern alembics?) to the notoriously inscrutable twentieth century "black boxes," of which the Institute has an enviable collection. As each selected, single artifact will be positioned just out of the reach of visitors, a first encounter with it will encourage initial engagement with its formal features and aesthetic dimensions and an appreciation of its "thingness" and auratic qualities.

This initial opportunity to visually appreciate the artifact will be augmented by multiple opportunities to explore and interrogate it through the provision, in the artifact's surround, of a diverse array of supplemental prompts and interpretive technologies. These prompts and technologies will run the gamut from low- to high-tech, inviting visitors to choose the learning/entertainment affordances with which they are most intrigued or comfortable: laminated cards with printed questions and answers; three-dimensional object replicas that can be opened and manipulated; smart phone- and tablet-based tutorials, digital animations, and augmented reality object overlays; and virtual reality projections and holograms. The technologies will vary and will provide visitors with answers to myriad questions about the featured artifact: What does it do? What theoretical or practical problem(s) was it designed to address? How was it manufactured? By whom? Who paid for it? What is it made of? What was, and is, its scientific, industrial, and/or monetary value? What technology(ies) preceded it? What technology(ies) followed it? Over time, an initial list of questions will be supplemented or replaced by others suggested by visitors, encouraging them to participate with curators in the process of interrogating, "unpacking," and making meaning from these artifacts (21).

This "360 degree" approach to investigating, understanding, and taking intellectual and aesthetic pleasure in a single artifact, no matter how inaccessible or unappealing it may appear at first glance, will be designed, it is hoped, to serve multiple purposes. It will, firstly, try to acquaint visitors with critical tools via exposure to a range of ways to "question" chemical artifacts. In so doing, it will help them develop conversance with perspectives that reflect the interests of scientists and historians of scientific innovation and discovery, as well as those of social historians and students of material culture.

It is also anticipated that, by taking time at the beginning of their visits to immerse themselves in a single artifact, visitors will learn to *slow down* their encounters with all the exhibits in the Institute's museum and, by extension, in other museums. People who have been conditioned (by years of visits to retail settings, as well as to museums) to traverse galleries rapidly, pausing only briefly to digest object labels or cast superficial glances at artifacts, may grow newly comfortable lingering over displays and engaging in critical explorations of their contents. They may learn, in a sense, to see less and yet see more, simultaneously.

Indeed, encouraging chemically curious visitors (as well as those initially indifferent to chemistry's charms) to "see more" will be an overarching aim of what we might call our "Gateway Artifact" project. Institute patrons who, upon arrival, are receptive to this multi-media, multi-valent exercise in looking and learning will be encouraged to regard all the chemical artifacts in our exhibits not as impenetrable objects but as gateways—portals into myriad avenues of inquiry and stories about chemistry's past and present. The goal will be to offer information and perspectives that intersect at least a few of the interests and life experiences that each visitor brings with them to the museum. In this way, we hope to provide interpretive models for our visitors' future encounters with chemistry's material culture, whether those take place in museums or via experiences of the chemistry embedded in their daily lives (22). We are optimistic that this project will be one vehicle through which the Institute (and our peer stewards of chemistry's history) can help "bring chemistry back" for museum audiences. By catalyzing a spirit of inquiry in our visitors, and spurring them to see our exhibits as useful points of departure for lifetimes of learning about chemistry, we aim to generate fresh interest in the history of this fascinating but obscure science.

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HISTORIOGRAPHY OF CHEMICAL INDUSTRY: TECHNOLOGIES AND PRODUCTS VERSUS CORPORATE HISTORY

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Abstract

In the twentieth century, the chemical industry was, in terms of innovation, among the most quickly changing of all industries. What remained constant, at least until the turn of the century, was its control by Western behemoths, such as Du Pont, ICI, and BASF. However, over the past two decades, driven by fragmentation and globalization, there has been a complete transformation of the industry. Thus Du Pont has merged with Dow, and ICI has ceased to exist. BASF remains one of the few survivors of the large, old corporations. The outcome is that historiography of chemical industry according to the model built mainly around these corporations has become complex, if not redundant. What if the historical analysis of corporations is shifted to an analysis of the interactions and transitions between technologies, within the industrial and global contexts, by revisiting and building on past achievements? Here such an approach is taken using as examples of industrial practice a single sector, synthetic ammonia: ICI's technologies, which includes manufacture of hydrogen, and the ceding of the role of high-pressure catalytic process plant design away from chemical companies to chemical engineering contractors. This enables a discussion of ICI's fall, and the complexity of what followed, to be tempered by the legacy of innovation in a sector that through the hydrogen economy is today receiving unprecedented attention.

In April 1986, the BBC's prestigious Richard Dimbleby Lecture was given by Sir John Harvey-Jones, chairman of Britain's Imperial Chemical Industries (ICI). The title of the lecture was, appropriately for the head of the nation's largest manufacturing conglomerate, "Does Industry Matter?" ICI, founded in 1926 as the result of a merger of four leading firms, was in the 1960s and until the early 1970s, in terms of annual sales, second after Du Pont in the league of global chemical manufacturers (1). In 1984, "ICI was the most profitable world chemical company." In 1986, as Harvey-Jones emphasized, ICI performed a vital role in the battle against Britain's widely perceived industrial decline: "ICI alone has a positive contribution to the tune of nearly £2 thousand million a year." Above all, "It is manufacturing industry whose praises I want to sing tonight." There was no other antidote to decline: "It is often suggested that tourism offers salvation. It is equally clear that this cannot be…. if we imagine the UK can get by with a bunch of people in smocks showing tourists around medieval castles we are quite frankly out of our tiny minds" (2).

In 1991, ICI trumpeted the fact that it was "one of the best-known names in the corporate world…. [and] is the most international of the world's chemical groups" (3). Today, ICI no longer makes a positive contribution to the UK economy. In the late 1980s, the corporation embarked on a period of major restructuring, caused by low margins, and often losses, in its cyclical bulk commodities, in part arising from increases in the price of energy (4). In the early 1990s, the management began to sell off the commodities businesses in order to invest in an ultimately expensive move into consumer products. The first major division to go was ICI's soda ash operation, divested in 1991 as Brunner Mond Holdings (and eventually acquired by Tata Chemicals of India in 2006). The nitrogen and fertilizer divisions followed soon after. In 1997, Zeneca, ICI's pharmaceutical spin-off, merged with the Swedish Astra to create AstraZeneca; ICI acquired Unilever's specialty chemicals business; and soon found itself with four billion pounds in debt. In early 2008, what remained of ICI was sold to AkzoNobel of Holland. ICI was completely defunct. No less significant was the fact that many of the once thriving core commodities businesses had been divested or sold off to foreign corporations. ICI, once a great success, had now become irrelevant. It seemed that Britain, at least until the arrival of Covid-19, was getting by with a bunch of people in smocks showing tourists around medieval castles, and contributions from the service industries. There was, however, a decade old, though then struggling, chemical corporation, Ineos, that had brought together commodity divisions from several other firms, including ICI's fluorochemical and chlor-alkali businesses.

ICI's disappearance was part of a pattern that was followed elsewhere in the chemical industry, though in many ways its total collapse was an extreme case (5). In common with ICI, many of the great chemical corporations that dominated the twentieth century had lifetimes of sixty or seventy years (apart from those broken up after 1945 in Germany and Japan). A few managed to survive, mainly intact, for considerably longer, before disconnecting with the past through closedown of traditional manufacturing processes, through mergers and acquisitions, or in response to environmental issues. Mergers were followed by de-mergers and spin-offs. Rivals acquired subsidiaries in order to support expansion. Moreover, corporate reconfigurations often entailed changing focus into biomedicines and specialties, and, as at ICI, research in "biology-based businesses" (3). In other cases corporations became less relevant, such as Monsanto, whose brand name was dropped shortly after it was subsumed by Bayer in 2018 as a result of campaigns by environmental activists against Monsanto's herbicides and genetically-modified crops.

Generally, the media today do not think much of the chemical industry, unless galvanized by stories of toxic releases, or, especially in the business columns, of corporate raiders, and activist hedge funds. "It has more to do with financial engineering than chemical engineering," wrote John Gapper in the *Financial Times*, on 1 June 2017, under the heading "Chemicals were the future once but no longer." Gapper opined that ".... there is not a great future in chemicals. If there were, then companies such as Dow Chemical, DuPont, Evonik, and ChemChina would not be involved in a series of mergers, the biggest wave of restructuring since conglomerates spun off their pharmaceutical divisions in the 1990s" (6).

While we may question perceptions and profiles of the chemical industry as appearing in the columns of the *Financial Times*, we cannot ignore the fact that in 2017 its readership exceeded 900,000, a significantly greater exposure than any history of chemistry/science/technology journal.

Nevertheless it is true that as a result of various transformations the long-standing heritage chemical industries of Europe and North America bear little resemblance to their standings in the seventy-year epoch that began around 1920 (Table 1). Which is why corporate changes at the turn of the century represent a form of closure of history of chemical industry as it had functioned in the past. This presents a number of challenges to historians of the industry, as does the fact that because corporate raiders play major roles in reformulating the chemical industry, researchers are already confronting the problem of reduced access to archival material in Europe and North America (unless disclosure is required in litigation). Other considerations apply to China and elsewhere. This begs the question: If historiography of chemical industry still matters, how do we pursue it in ways that are different from the past when it was possible to write histories of the great firms during the relatively stable period? Here I would like to consider the prospects for an integrated history of the modern chemical industry by examining a group of important chemicals through their modes and scales of manufacture, and their impacts on certain world affairs, rather than through the complexity of corporate changes.

I take as the starting point ICI's storied vast synthetic ammonia facility at Billingham, in northeastern England, which commenced production of ammonia in 1924 after imitating the BASF Haber-Bosch process (1913), itself a massive endeavor and the template for all subsequent ammonia processes (7). By the 1960s, when ICI was the largest producer of ammonia in the world, it operated four other ammonia facilities: Heysham (constructed for the Ministry of Supply during World War II), Wilton (1949; ammonia production began in 1952), Severnside (1963), and Immingham (1966). By the 1980s, there were eight ICI ammonia facilities. ICI's engagement in the relevant technologies, including novel high-activity catalysts, and two low-pressure ammonia processes, had an almost mythical provenance, at least among chemical

Table 1. Examples of Amalgamations, Mergers and Independent Firms in the European and US Chemical Industries

20th-Century Mergers	
1917	**Union Carbide and Carbon, USA**
1920	**Allied Chemical & Dye, USA. AlliedSignal 1985; Honeywell 1999**
1925	**IG Farben, Germany**. Dismantled after 1945, to form **AGFA**, **BASF**, **Bayer** and **Hoechst**. AGFA is a subsidiary of **Bayer**
1926	**Imperial Chemical Industries** (ICI), **UK**. Alkali division divested, as **Brunner Mond 1991**. Demerger of pharmaceutical and agrochemical divisions to form **Zeneca 1993**. Zeneca merges with **Astra**, Sweden, to form **AstraZeneca**, **1997**. Other divestments discussed in text
1928	**Rhône-Poulenc, France. Société *Chimique des Usines du* Rhône** merges with **Établissements Poulenc Frères**
1929	**American Cyanamid and Chemical Corporation, USA. Cytec,** chemicals, spun off **1993-94;** life sciences, agrochemicals and consumer products to **American Home Products (Wyeth) 1994**
1966	**Montecatini** merges with **Edison** to form **Montedison, Italy**
1970	**Ciba-Geigy, Switzerland.** Renamed **Ciba 1992.** Merges with **Sandoz** to form **Novartis 1996**
1994	**AKZO** merges with **Nobel, Netherlands**
1999	**Hoechst** merges with **Rhône-Poulenc** to form **Aventis**

Major Independent Firms at the Close of the 20th Century
Bayer, Germany **Ineos, UK (founded 1998)** **BASF, Germany** **Monsanto, USA** **Dow, USA** **Solvay, Belgium** **DuPont, USA**

21st-Century Mergers	
2001	**Union Carbide & Carbon** to **Dow**
2004	**Aventis** merges with **Sanofi-Synthélabo** (**Sanofi**), **France**
2007	**Evonik,** merger of German firm **Lyondell Chemical** to **Basell Polyolefins** to form **LyondellBasell, USA/UK**
2009	**Rohm and Haas** to **Dow**
2017	**DuPont** merges with **Dow,** to form **DowDuPont**
2018	**Monsanto** to **Bayer**

engineers. This, however, has received scant attention from historians of chemical industry.

Synthetic ammonia was one of ICI's most important commodities, and though not always profitable, was essential to agriculture. In the 1990s, the corporation's divestment program involved disposal of its ammonia and nitrogen fertilizer units. Their subsequent ownerships, and the eventual consolidation in 2015 as part of CF Industries, of Illinois, today the world's largest manufacturer of ammonia, are shown in Table 2.

This illustrates well how, as in other sectors, unfamiliar names emerged on the way to consolidation. For the historian interested in the chemical industry of the recent past the changes are undoubtedly a source of confusion. We are not dealing with changes in divisions and departments here, but completely different corporate entities. In just over two decades there had been more changes of ownership at ICI's ammonia business than in the previous seven decades. And there was not a great deal to show in the way of technical innovation.

Synthetic ammonia, as a high tonnage chemical, presents itself as an example for a new approach to a broader understanding as to why the chemical industry is not only vital but makes necessary the need for historians to record its processes and products. This includes the study of feedstocks, energy needs, and process improvements, in addition to research, design, and engineering, and the changing structure of the industry.

Framed within the challenge of nitrogen fixation, synthetic ammonia is accorded a major role in the feeding of humanity, and thus in its growth and expansion. What is less well appreciated is that success is conditioned on production of pure hydrogen in order to prevent catalyst poisoning. ICI happens to hold a special place through its

Table 2. Towards Consolidation in the British Ammonia Industry. Corporate Ownership of Billingham and other Ammonia Factories

1920-1923	Brunner, Mond & Co. develop ammonia synthesis.
1924	Brunner, Mond & Co. produce ammonia at Billingham.
1926	(December 7) ICI (Imperial Chemical Industries) created from merger of Brunner, Mond with Nobel Industries, British Dyestuffs Corporation, and United Alkali.
1965	Shellstar (Shell/Armour Star) ammonia factory opens at Ince, Cheshire, northwest England.[a]
1975	Ince sold to DSM of Holland. Trades as UKF.
1985	Ince sold to Kemira Oyj, of Finland, whose agricultural unit becomes Kemira Agro Oy. Kemira also acquires an ammonia plant at Hull.
1990	ICI pursues options to divest of ammonia operations.
1991	Terra Nitrogen (UK) Ltd, part of Terra Nitrogen Company, of Deerfield, Illinois (founded in 1991), purchases ICI Billingham and Severnside fertilizer ammonia facilities.
2004	Kemira Agro Oy spun off as Kemira GrowHow Oyj.
2006	Terra and Kemira GrowHow Oyj form 50-50 joint venture, GrowHow.
2007	Kemira GrowHow acquired by Yara International (formerly part of Norsk Hydro) of Norway. Ince modernized.
2010	Terra, and its share in GrowHow, sold to CF Industries, of Deerfield, Illinois (founded in 1946 as the Central Farmers Fertilizer Company).
2015	Yara's UK share in GrowHow sold to CF Industries. GrowHow rebranded as CF Fertilisers in November.

[a] The Shellstar factory is included because of the connection with Kemira Oyj. Severnside closed in 2008.

contribution to the complete range of hydrogen generation processes from fossil fuels: from coal by the water gas process, and from naphtha, natural gas, and other hydrocarbons through the process of steam reforming.

Hydrogen

Water Gas, Coking Oven Gas and Electrolysis

Until the 1940s, the main processes for large-scale production of hydrogen were based on coal. ICI manufactured hydrogen by imitating BASF's technology. Red hot coke was treated with steam in gas generators to give water gas, a mixture of carbon monoxide and hydrogen, from which the contaminant hydrogen sulfide was removed using iron oxides. The carbon monoxide was then converted into carbon dioxide by the water gas shift reaction. The shift reaction also gave more hydrogen. The carbon dioxide was scrubbed out with water, and any remaining monoxide was absorbed in a solution of cuprous ammonium formate.

$$C + H_2O \leftrightharpoons CO + H_2 \qquad \Delta H\ +118.7\ \text{kJ/mol}$$

$$CO + H_2O \leftrightharpoons CO_2 + H_2 \qquad \Delta H\ –42.1\ \text{kJ/mol}$$

water gas shift reaction

This was followed by the ammonia synthesis, at a pressure of around 250 atmospheres, in the presence of a magnetite-based catalyst, and at an elevated temperature. The yield was around 5-8 %.

$$3\ H_2 + N_2 \leftrightharpoons 2\ NH_3 \qquad \Delta H\ – 91.8\ \text{kJ/mol}$$

The other main hydrogen process drew on coking oven gas, which is rich in hydrogen, as widely adopted in Europe from the mid-1920s. This source also required extensive purification. Where cheap hydro-electric power was available pure hydrogen was produced in electrolytic cells, mounted in electrolyzers, but in most cases the electricity was too expensive. At the end of the 1920s, the introduction of synthetic methanol created even greater demand for hydrogen, which when generated with carbon monoxide became known as synthesis gas (syngas), and was a cornerstone of many manufacturing processes.

Steam Reforming of Hydrocarbons

ICI's most original contribution to production of hydrogen prior to 1940 was in steam reforming. This started with international interest in synthetic gasoline made by hydrogenation of coal, based on the Bergius process of IG Farben in Germany. In the United States the process was investigated by Standard Oil of New Jersey. However, interest in hydrogenation of coal to provide liquid fuels declined in the United States because of the discovery of large deposits of petroleum. This was not the case in Britain, nor in Germany.

The steam reforming process consists of heating hydrocarbons in the range 700-1100 °C in the presence of steam and a nickel catalyst. Hydrogen and carbon monoxide are formed, as in the water gas reaction. In the case of natural gas (methane):

$$CH_4 + H_2O \leftrightharpoons CO + 3\ H_2 \qquad \Delta H\ +206\ \text{kJ/mol}$$

The most advanced steam reforming plant for manufacture of hydrogen was developed at ICI from 1928. It operated at atmospheric pressure and was installed at Billingham for the ammonia process in 1936. In this case the propane/butane byproducts of coal hydrogenation were reformed to hydrogen. Significantly, this was then of no interest in Germany, which relied on abundant lignite (brown coal), nor in the United States, where there was a growing interest in reforming of natural gas (7, pp 112-113). However, ICI's work was a precursor to the modern methods of reforming liquified petroleum gas (LPG, a mixture of propane and butane).

When after 1940 the United States embarked on expansion of ammonia production for strategic purposes, six of the ten new government-backed plants relied on ICI's process for the steam reforming of natural gas. It was this novel way of producing hydrogen that provided an early opportunity for engineering contractors to enter into the manufacture of synthetic ammonia. From the 1960s, these firms became front runners in the development of new hydrogen and ammonia technologies. Where natural gas was abundant, notably in the United States and Italy, it became the main source of hydrogen for ammonia by the end of the 1940s. In Britain methane was available from coke gasification, but this made it expensive as a feedstock. In Germany, where there was a considerable demand for methane for use in the manufacture of acetylene by the electric arc process, the methane was mainly available from coking ovens gases.

Hydrogen from Naphtha

For hydrogen, ICI relied on hard (bituminous) coal that was, apparently, less well suited to the water gas reaction than the lignite used in Germany. As an alternative feedstock for the ammonia process, ICI's chemists-engineers in the 1950s investigated oxygen gasification of fuel oil, and, at around the same time, the ultimately more successful steam reforming of low-sulfur naphtha, a mixture of light distillate hydrocarbons. They developed a naphtha-based synthesis gas process using pressurized steam reforming and catalysts that prevented poisoning with sulfur and the buildup of carbon in the reformer tubes. In 1959-1960, this steam reforming process was introduced on a commercial scale at Heysham, in 1962 at Severnside, and in 1963 at Billingham. It was the *first ever* large-scale application of pressurized steam reforming to liquid hydrocarbons. In order to extend the life of the furnace tubes, a second reforming stage was introduced in which unconverted hydrocarbon was oxidized. In secondary reforming, a process earlier developed by ICI, the partially reformed hydrocarbon is reacted with air, which at the same time provides the nitrogen for the ammonia process (8). Secondary reforming was followed by heat recovery, a two-stage carbon monoxide shift reaction, and removal of carbon dioxide by washing with hot potassium carbonate solution.

Recovered carbon dioxide was used in the manufacture of urea, an increasingly important fertilizer, by reaction with ammonia, and also sold to the beverage industry. By the mid-1960s, ICI's two-stage pressurized reforming process was licensed to six leading international engineering contractors, including M.W. Kellogg in the US, and Humphreys & Glasgow in the UK (9). In the 1970s, the process was readily adapted to reforming of North Sea natural gas.

$$CH_4 + 2\ O_2 \leftrightharpoons CO_2 + 2\ H_2O \qquad \Delta H\ –35.6\ \text{kJ/mol}$$

secondary reforming

$$CO + H_2O \leftrightharpoons CO_2 + H_2 \qquad \Delta H\ –42.1\ \text{kJ/mol}$$

water gas shift reaction

This brought to an end the use of coal as feedstock in the ammonia industry in Britain. ICI was also a leader in synthesis of methane by steam reforming of naphtha which, along with hydrogen from naphtha, around 1970 aroused considerable interest in the United States where there were concerns over a shortage of natural gas.

From the 1960s, the technology of ammonia production increasingly relied on a change in design philosophy, involving a more holistic approach based on a total-unit-based integrated concept, rather than on a conventional, interdependent, kit of parts, as taken by engineering contractors, in particular M. W. Kellogg. ICI's work on steam reforming under pressure was critical to Kellogg's reconfiguration of synthetic ammonia technology.

M. W. Kellogg's Single Train Ammonia Unit

The synthetic ammonia industry was transformed with development in 1963 of the single-train energy-integrated ammonia unit, powered by a centrifugal compressor. It enabled production of 1,000 tons a day of ammonia in a single synthesis loop. This tripled the output obtained with loops using the previously standard reciprocating compressor (10). The first design was drawn up by Kellogg, then of New York, for ICI's Severnside factory. Though Kellogg did not receive an order from ICI at that time, because catalyst calculations took longer than anticipated, this represents one of the high points in the shift from innovations in the chemical industry over to engineering contractors. Moreover, its success relied on ICI's developments suited to full-scale pressurized steam reforming. Kellogg installed the first pressurized steam reforming unit for ICI, at Heysham. This contributed towards Kelloggs's appreciation of ICI's reforming technology. The reforming process brought about significant savings by integrating heat energy and the energy required for gas compression. It almost completely obviated the need for additional inputs of steam and electricity. The process was a critical component of Kellogg's design of the single-train process (11). In 1964, Kellogg, now in a position to provide catalyst performance data, received a contract from ICI for construction of three single-train units at Billingham.

Versions of the single-train unit were soon after designed by other engineering contractors (for a time Kellogg claimed priority, based on pilot plant studies undertaken in the 1950s). ICI, though maintaining research into synthetic ammonia and related processes, including high-activity catalysts, increasingly outsourced design and erection of its plant for bulk commodities to engineering contractors, including Bechtel, Kellogg, and Humphreys & Glasgow.

The new reformer and single-train ammonia technologies had a major impact in India, and, once the United States opened up to business with the main communist powers, in China and Russia. The technologies of nitrogen products, and also of methanol, became tools of international diplomacy; their global transfers were brought about through engineering contractors, cross-licensing of technologies, and international financing. This was the beginning of a new era in the history of chemical industry, one that has little to do with the traditional Western corporations. Nevertheless its success was an outcome of ICI's pressurized steam reforming technology as integrated into Kellogg's single-train process.

India: Ammonia for a Developing Economy

The global map of the synthetic ammonia industry changed with the emergence of the so-called Green Revolution, in the mid-1960s, which relied on new hybrid high-yield varieties of wheat and rice, and nitrogen fertilizers. This enhanced the transition of sites of production from Western countries and Japan to locations close to areas of consumption (12).

From the end of 1965, the United States and World Bank encouraged India and Pakistan to accept assistance from Western multinational engineering contractors in developing large-scale nitrogen fertilizer industries (13). While the plant installation costs were high, it was emphasized that home-produced ammonia and nitrogen fertilizers would remove the need for valuable foreign currency to pay for imports of much needed grain. The situation became critical as the result of a severe drought in 1966.

In the same year, ICI's naphtha steam reforming process was adopted in a new 500 mtpd (metric tons per day) ammonia plant for Gujarat State Fertilizer Co. Ltd, on the west coast of India, constructed by Humphreys & Glasgow and Japan's Hitachi-Zosen (14). In 1969, ICI's synthetic ammonia technology was introduced at Kanpur (Uttar Pradesh); the ammonia was converted into urea by the process of Japan's Toyo Engineering. Also in 1969, Japan's Chiyoda Chemical Engineering & Construction was appointed lead contractor for an ammonia-urea project at Kota, Rajasthan, in the northwest of the country, incorporating processes licensed from European and American firms (10, pp 136-137). Kellogg designed and constructed the first large scale, natural gas fed, all-centrifugal ammonia unit in India, at Kalol, Gujarat, for Indian Farmers Fertiliser Cooperative. It was part of a 120-million dollar ammonia fertilizer complex, producing urea and NPK fertilizers, formally opened by Prime Minister Mrs Indira Gandhi on 8 November 1974 (15). Finance came from the United States Agency for International Development and the United Kingdom Overseas Development Association.

With the support of Indian-made nitrogen fertilizer, the increase in food grain yield enabled India to become self-sufficient in wheat, and no longer to rely on imported rice. Significant, for long-term growth, was the know-how transfer to Indian scientists and engineers (16). Indian food production rose from 50 million metric tons in 1950-1951 to 152.4 million tons in 1984-1985 (17). In Pakistan during 1975, Kellogg began construction of a 900 mtpd single-train ammonia plant, financed by the International Bank for Reconstruction and Development (18). Ammonia factories had become the front line against hunger and malnutrition.

Western Firms and China

When in the 1970s, Western chemical and engineering contractors were badly hit by the economic impact of increased energy prices and competitive pressures they found some relief in the shape of the growing markets in Asian and Eastern Bloc countries. The People's Republic of China was of particular significance to American contractors. In 1971, at the mid-point of the Cultural Revolution (1966-1976), China became interested in trade with the United States. President Nixon was then dealing with major problems in the American economy and the war in Vietnam. Industries were encouraged to increase exports, in order to support the dollar, and to explore new markets. The US administration hoped that by opening up to China it might be possible to take advantage of frictions between China and the Soviet Union, then the main backer of North Vietnam, in order to bring pressure to bear on the Russians, which could in turn be used to help bring about an end to the war. Nitrogen fertilizer plants were among the main bargaining tools.

In February1972, Nixon travelled to China to meet with Mao Zedong and Premier Zhou Enlai. The Chinese government soon after ordered thirteen large ammonia-urea complexes, of which eight were assigned to Kellogg, and five to European and Japanese firms. The Kellogg order, for 1,000 mtpd single-train ammonia units, represented "the largest dollar volume [order] ever placed by the PRC with a U.S. firm in the industrial sector" (19). Moreover, the combined size of the Chinese orders was unprecedented in the history of chemical industry.

By 1986, as a result of the importation of Western ammonia technologies, there were fourteen ammonia plants operating with rated capacities of 1,000 mtpd, and three more under construction. China, by building world-scale ammonia plants, became the global leader in ammonia production in the early 1990s. China also emerged as an important innovator. An example, in the context of this paper, is a high activity novel catalyst for the ammonia synthesis based on wüstite ($Fe_{1-x}O$) discovered in the 1980s at Zhejiang University of Technology (20). The technology was licensed to Süd-Chemie in Germany; production of what were called Amo-Max® catalysts commenced in 2003. Billingham was one of the users of this catalyst. This represented a major departure from the traditional magnetite catalysts that had been used over the previous century.

The Soviet Union

From the late 1960s, developments in the Soviet Union paralleled those in China. At that time, European firms were already open to direct business with Soviet and Eastern Bloc enterprises. To obtain a foothold in these markets, Kellogg engaged in partnerships, licensing, and other arrangements with Japanese and European engineering contractors. In 1969, Kellogg provided Japan's Toyo Engineering with the process design for a 1,500 tpd ammonia unit at a fertilizer factory located in the foothills of the Caucasus Mountains. It went on stream in 1973.

The large Eastern Bloc market was a factor in Kellogg's acquisition in January 1973 of 51% of the Dutch firm Continental Engineering from Verenigde Machinefabrieken (VMF). Continental Engineering, renamed Kellogg Continental BV, opened up the market for Kellogg ammonia technology in the Soviet Union (21). Process design was licensed through Kellogg Continental to Toyo Engineering, which with Soviet engineers erected five plants in Russia (22). In June 1974, the engineering contractor Chemico (a former division of American Cyanamid) signed a $200 million contract for construction of four ammonia facilities on the Volga River. Funding for these factories was provided by the Export-Import Bank of the United States, the official export credit agency of the US government (23).

The Energy Crisis

The change in the scale of ammonia production resulting from new technologies included process efficiencies that enabled a substantial reduction in the use of natural gas, as the result of the introduction of pressurized reformers and centrifugal compressors (7). Quite unexpected, however, were events in the 1970s that would upset the world energy balance.

Between late 1973 and early 1975, in the wake of the Yom Kippur War, the free market economies suffered from the almost fourfold increase in the price of hydrocarbons. This, however, had little impact on orders for ammonia plants from countries with central and regional planning, notably China and the Soviet Union. The *Wall Street Journal* in December 1974, under the heading "No slump here: builders of ammonia plants benefit from global demand," emphasized the fact that American engineering contractors were engaged in twelve ammonia projects in the Soviet Union, nine involving Kellogg and three Fluor Corporation, of Los Angeles, in addition to eight projects in China (24).

In 1976, Kellogg, by then moved to Houston, signed a contract for supply of a 1,500 tpd synthetic ammonia unit to the Soviet Union, bringing to eighteen the number of Kellogg designed ammonia plants operating in, or contracted for, Russia (25). At the same time, Montedison's engineering division, Tecnimont SpA, received an order from the Soviet Union for a urea plant of 500,000 tons annual capacity (26). These plants contributed greatly to the Soviet Union's role as the leading global producer of synthetic ammonia until around 1990, when it was overtaken by China.

Significantly, in the 1970s the Middle East countries were emerging as major producers of ammonia, drawing on natural gas and Western technologies. In Iran during 1970, Kellogg completed a petrochemical complex incorporating a 1,000 tpd ammonia unit; a second unit was installed five years later (27). In the mid-1970s, the Saudi Arabian Fertilizer Company (SAFCO) commenced large-scale manufacture of ammonia and urea (28). Regime changes, and in the early 1980s a drop in the price of oil, did however cause difficulties for Western engineering contractors, resulting in bankruptcies, takeovers, mergers, and consolidations.

ICI's Catalysts

The 1970s and 1980s saw several major improvements in the technologies of high-pressure catalytic processes. In steam reforming, ICI's nickel catalysts enabled increases in the pressure, permitting use of even fewer tubes, which were made of expensive alloys, and smaller furnaces. Heat was recovered for use in other sections of the ammonia unit (29). Iron oxide and copper catalysts were used in the shift reactions. A nickel catalyst brought about more efficient removal of carbon oxides from synthesis gas by methanation, a process introduced in the 1960s.

$$CO + 3\,H_2 \leftrightharpoons CH_4 + H_2O \qquad \Delta H\ {-206.1}\ \text{kJ/mol}$$

$$CO_2 + 4\,H_2 \leftrightharpoons CH_4 + 2\,H_2O \qquad \Delta H\ {-164.9}\ \text{kJ/mol}$$

In the mid-1970s, ICI invested two million pounds sterling on extending its catalyst division, known as ICI Katalco, for manufacture of hydrogen, ammonia, and methanol catalysts. New catalysts, along with the introduction of centrifugal compressors, enabled large plant throughputs in both ammonia and methanol under milder conditions.

An important ICI contribution to the Soviet Union's chemical industry was a low pressure methanol process which, using novel high-activity catalysts, reduced the operating pressure from 300 atmospheres to 30 to 120 atmospheres. There were also considerable savings in consumption of feedstock. The process, introduced in 1968, was in use at Billingham from the mid-1970s (30). Contracts for two methanol plants were drawn up with Russia in the summer of 1977. Finance came through a buyer credit arranged by Morgan Grenfell Ltd, under the terms of the 1975 Anglo-Soviet Credit Agreement. The plants, at Gubaha in the Urals, and Tomsk, in Siberia, were the largest methanol facilities in the world, and represented Britain's largest ever deal with the Soviet Union. This brought to 26 the number of facilities that worked the ICI methanol process, which accounted for some 80% of world capacity (31).

ICI's active catalysts contributed to the development of a new, lower energy ammonia process at Billingham. It was called Ammonia V, abbreviated to AMV, and developed by 1984. The process featured a low-pressure synthesis loop, operating at about 80 to 110 atmospheres, half the pressure generally in use until the 1960s (32). It employed, for the first time, a cobalt-promoted high-activity synthesis catalyst (Katalco74-1) (Table 3) (33).

Though the same basic process was common to other new designs developed in the 1980s, the operating conditions were different (Figure 1).

Unfortunately for ICI, depressed economic conditions were impacting on all sectors of the economy, no less the synthetic ammonia industry. As a result, the AMV design was not adopted at Billingham. The first prototype was put into operation in August 1985 at the Nitrogen Products Factory (formerly CIL, Canadian Industries, Ltd), at Courtright, Ontario, Canada.

However, ICI's Severnside facility, with its then two ageing units, was modernized, using the corporation's new Leading Concept Ammonia (LCA) process, announced in 1988. It employed catalysts enabling even lower operating pressures than the AMV process, that is, between 70 and 80 atmospheres. (ICI's LCA and AMV processes had been developed under the guidance of Alwyn Pinto.) In the redesign of the steam reforming process, the primary reformer was arranged to receive heat from the process gas exiting the secondary reformer. This concept, proposed by Chiyoda in 1984, did away with the need for a primary reformer furnace. The LCA process was suited to ammonia units of relatively low daily capacity, for which there was still demand, and

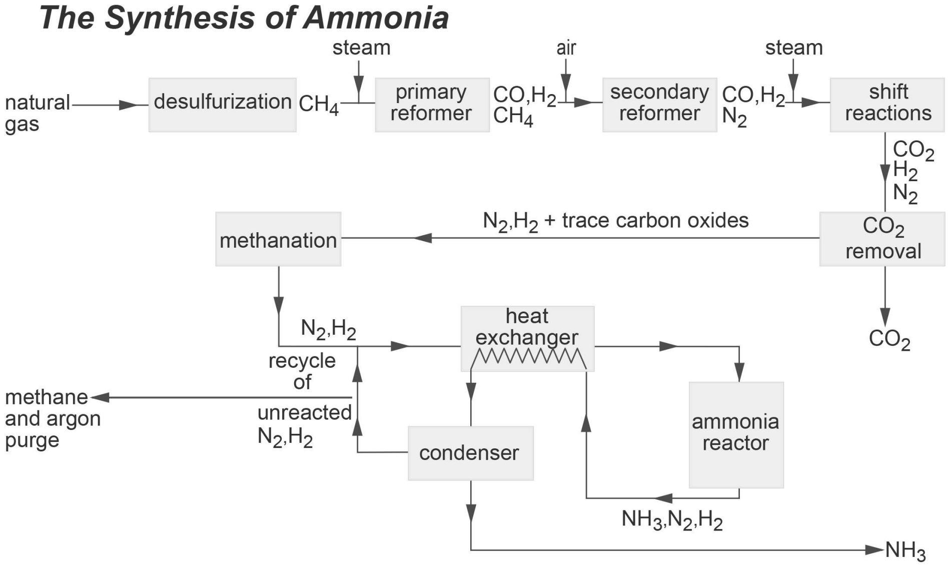

Figure 1. *Ammonia synthesis from natural gas, at ICI Billingham, 1970s.*

with a yield of 12 to 15% compared favorably with other processes.

By 1990, ICI ammonia production had been losing money for four years. Rather than use its advanced technology to improve the ammonia units at Billingham, ICI decided to dispose of its ammonia facilities. ICI, however, continued to license the LCA process, and remained in the catalyst business. In September 1990, the catalyst unit, ICI Katalco, became Katalco. In 1997, Katalco purchased BASF's synthesis gas catalyst division. Five years later, Katalco was acquired by Britain's Johnson Matthey, which has continued to develop novel catalysts at Billingham.

The foregoing account is no more than a fragment of the modern industrial ammonia story. From the 1980s, the high cost of installing new plant stimulated a sector based on plant upgrading, including redesign of converter internals, as well as improved reformer technologies, offering not only higher capacities but even greater savings in energy. More recently, designs have been drawn up for ammonia units with capacities of up to six thousand tons a day, based on sustainable ammonia production. Steam reforming of natural gas remains the dominant process for manufacture of hydrogen, with, increasingly, moves towards complete carbon capture. In the long term, electrolysis of water, drawing on wind and solar power, is expected to rival steam reforming. Both processes are critical to the emerging hydrogen economy, now focused on energy production, in particular the much-lauded fuel cells, and the use of hydrogen as an energy carrier. Ammonia and hydrogen have a long shared history that promises much for the future, and for the future historian of chemical technology. But it is no longer a story of Western corporations alone.

Conclusion

The history of the modern chemical industry is not unlike larger national histories in that it refracts a complex story of how major but sometimes lesser known challenges are met. A case in point is ammonia production, including of hydrogen, in which ICI, notwithstanding its disappearance, played a prominent role. ICI's connection with ammonia is certainly less chronicled than the corporation's remarkable range of science-based innovations, including phthalocyanine and fiber-reactive dyes, polyethylene, Perspex, and beta-blockers and other cardiovascular drugs used to treat high blood pressure.

Table 3. Examples of ICI Katalco Catalysts Developed for the Synthesis of Ammonia (33)

Katalco 61-2	The first low-temperature hydro-desulfurization (HDS) catalyst
Katalco 83-1	The first application of a process gas heated reformer (GHR), isothermal shift catalyst developed to resist the high operating temperature
Katalco 11-4	A low-temperature methanation catalyst
Katalco 74-1	A cobalt-promoted high-activity synthesis catalyst suited to the low pressure process for naphtha or natural gas

ICI has deserved our attention not just because it was a bastion of British industry. It was an example of in-house major innovations, of competitive advantage, of growth, and in the end of contraction. ICI was once a household word, and for many a mirror of the state of a nation. As Carl Mortished wrote in May 2018 in the London *Evening Standard* (34):

> In the old days, there was a very large enterprise called Imperial Chemical Industries, later stream-

> lined to ICI. The company did what it said on the tin, manufacturing chemicals and some consumer products, notably Dulux paint.
>
> It was so big that newspaper scribblers dubbed it 'the bell-wether of British industry'; stockbrokers and fund managers hung their investment decisions on its very utterance.
>
> ICI is no more; outgunned and outclassed by smarter, more efficient German, US and Far Eastern rivals. Today the fortunes of a company that publishes an online scrapbook command a lot more international attention than the likes of BASF, Dow Chemical and Britain's Ineos, but the chemical industry still tells us very important things about the state of the economy.

While the legacy businesses and their offshoots have lost their glamour in the digital age they, or their reincarnations, are still essential. Most, unlike ICI, were hardly known outside the chemical industry. Around three decades ago, as the chemical industry was expanding in Asia and the Middle East, several of the venerable Western firms, set in their ways, were cumbersome, and unwieldy. They had lost direction. The reasons are varied. Company scientists draw attention to the neglect of research, and innovation, as diversification accelerated in directions far removed from core interests, which pulled some firms down. This was certainly the case at ICI. In 1994, ICI, rather than choose a leader within its ranks with knowledge of the manufacturing divisions, appointed an executive from Unilever. The commodity manufacturing units continued to be sold off, but at far lower prices than expected, which left the corporation in serious debt (35).

ICI epitomizes the rise and fall of Western chemical firms, a theme that has attracted a great deal of attention, in particular from business historians. According to standard accounts, which take the story until around the year 2000, mergers of powerful firms gave way to monopolies, which created barriers to entry of new innovative firms. From the 1970s, when there was a perceived lack of innovation in the chemical industry, several firms used their immense capital and logistics networks, including in research and development, to diversify into pharmaceuticals (36). They subsequently divested of subsidiaries that dealt in bulk commodities, or no longer undertook research into improving manufacturing processes (Here, however, ICI's ongoing research into the ammonia process was an exception).

Less attention has been paid to the fact that this created opportunities for the entry of new players. A different form of chemical industry emerged, as represented by the UK's Ineos, which acquired two of ICI's commodity chemicals businesses in 2001, and BP's Innovene, an olefin and refining division, in 2005. By 2008, Ineos had acquired twenty-two companies; and went on to engaged in strategic and international partnerships. In other cases, failing or moribund firms reinvented themselves. Here, and relevant to this account, is the example of the Swiss firm Ammonia Casale, which from 1980, under a new leadership of experienced chemists and engineers offered a revamping (retrofitting) service to the ammonia industry. Its success led to advanced converter and reformer designs. Today, Casale (Ammonia Casale until 2014) is a leader in the technologies of nitrogen products, including in development of novel catalysts. Jointly with the Swiss firm Clariant (which acquired Süd-Chemie in 2011), Casale developed a highly active variant of the AmoMax® 10 catalyst, for which the two firms received the 2021 Sandmeyer Award of the Swiss Chemical Society.

No doubt, accelerated structural trends in chemical industry will continue as firms adapt to suit different needs. Despite the upheavals, changes in chemical technology remain relevant, even if often incremental, driven by sustainability, and environmental considerations.

The foregoing account offers a way of navigating the historiography of the recent past. It suggests a new way of thinking about industry by focusing on processes and products, and how they reach the marketplace, rather than by trying to make sense of the bewildering array of corporate fragmentation patterns and rearrangements. It requires a synthesis of contrasting approaches and perspectives, and a need to connect and harmonize with the past. Themes include sources of feedstocks and energy; the environment; international financing for large projects; the global reach involving transfer of scientific and technical skills from Europe and North America; joint studies between corporations and academic institutions; control and licensing of patents; the role of engineering contractors; and political and trade policies. Certain of these elements appear in the still evolving story of synthetic ammonia. The approach also represents a way of overcoming the boundaries created by the complexities of corporate changes. And in some ways even of explaining those changes.

Perhaps one could argue that while approaches to the post-twentieth-century history of chemical industry might not matter as much as in the past, in the way that has so far appealed to and constrained historians, the history of industrial processes and products is a completely different matter. Understanding process changes and their implementations provides a clearer appreciation of how and why innovations appear and change over time, and, indeed, why historiography of chemical industry has a future. Until now the historical studies have been the domain of scholars from the United States and Europe (37). In the future, as synthetic ammonia illustrates, they will need to create partnerships with their peers elsewhere, including chemists, economists, business historians and political scientists. One thing is certain: history of the chemical industry, in particular of its processes and products, and their expanding new uses, including, for hydrogen and ammonia, in the new "Chemical Century," still matters, especially if we wish to understand the recent past as a guide to the future.

Postscript

In mid-September 2021, high natural gas prices led to widespread cutbacks in the European ammonia industry. Manufacture in Britain ceased. With state support, at least until January 2022, the Billingham ammonia factory restarted production in order to ensure a continuous supply of food grade carbon dioxide (the by-product of reforming), of which it is the UK's main source.

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A FUTURE HISTORY OF SELECTIVITY IN ORGANIC CHEMISTRY: WHENCE, WHERE AND WHITHER?

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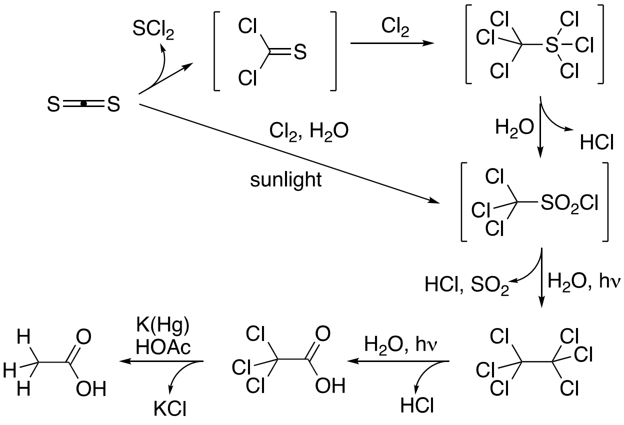
Abstract

A series of historical snippets of milestones in the development of selectivity in organic synthesis is presented, followed by a few prognostications about future directions in selectivity in organic synthesis—contingent on the cautionary observation that major advances are not always recognized as such at the time. The historical snippets include the foundational landmarks: the unambiguous synthesis of acetic acid from only inorganic substances by Kolbe, the Structural Theory by Couper and Kekulé and its modification by Butlerov in 1861, and the tetrahedral carbon of van't Hoff and Le Bel. Physical chemists and physical organic chemists provided insights into rates and mechanisms of reaction. In the space of a century and a half, organic synthesis had passed through eras of chemoselectivity, regioselectivity, and diastereoselectivity, to enantioselectivity. Along with advances in spectroscopy and separations techniques, the rise of computational chemistry has added yet another tool to the arsenal of organic chemists.

Defining the concept of selectivity was not one of the first fundamental questions identified by organic chemists. The reason is simple: until the development of a good theoretical footing, the appropriate questions could not be formulated. In 1840, for example, many organic chemists were preoccupied with obtaining evidence to support the legitimacy of the new science, including evidence that organic compounds could be prepared from demonstrably inorganic precursors. Those who already accepted the new discipline, saw the exploration of organic chemical reactivity as the prime task. The formal synthesis of acetic acid from its elements (Scheme 1) by Hermann Kolbe (1818-1884, Figure 1) (1) satisfied the former, but his accomplishment was only possible because of the results of other organic chemists whose exploration of organic reactivity yielded useful reactions such as the reduction of trichloroacetic acid with sodium amalgam, following Melsens' procedure (2). Its reducing power and ease of handling had quickly made sodium amalgam a popular reducing agent. Even this reagent had a debt to earlier chemists: by applying the Voltaic pile (3), which had been developed by Alessandro Volta (1745-1827, Figure 1), Humphry Davy (1887-1829, Figure 1) made metallic sodium available in 1808 by electrolysis of molten sodium hydroxide (4).



Scheme 1. *Kolbe's synthesis of acetic acid (depicted in modern structures).*

Davy Volta Kolbe

Figure 1*. Scientists whose combined work provided the evidentiary basis for the legitimacy of organic chemistry as a new subdiscipline of the science.*

The continued probing of organic reactivity ("What will react *with* what *to give* what?") did give a diverse set of useful reactions by the middle of the nineteenth century. But… until the Structural Theory of Organic Chemistry emerged in 1858-1861, there was no framework for the systematic interpretation of the results of these experimental observations.

A major problem for early organic chemists was that the amount of information conveyed by the formulas then in use was very limited. Organic chemistry's growth and the development of concepts such as "selectivity" required a representation that would show more granular detail than the Type formulas then in use. At the same time, the atomic weights of the elements also caused their own problems—until the Karlsruhe conference, most organic chemists used equivalent weights (C = 6, O = 8, S = 16, etc.), which led to confusing doubled atoms for these elements. In 1843, Gerhardt had proposed that doubling the atomic weights then in use would eliminate the double atoms of elements such as carbon, oxygen and sulfur, and so on (5). In his 1857 paper (6), August Kekulé (1829-1896, Figure 2) adopted Gerhardt's values for the atomic weights (H = 1, C = 12, N = 14, O = 16, S = 32, etc.), indicating this by means of "barred" symbols (~~H~~, ~~C~~, ~~N~~, ~~O~~, ~~S~~, etc.), and gave evidence for the tetravalency of carbon, atomic weight 12. This change in symbology has been discussed in more detail by Rocke (7).

This paper presents snippet views of some milestones in the development of selectivity in organic synthesis from the advent of structural theory to recent catalytic approaches to asymmetric synthesis. The stories of several of these milestones have been told in more detail elsewhere, while others merit more detailed and contextualized study. This paper ends with a few prognostications about future directions in selectivity in organic synthesis.

Whence?

The Structural Theory of Organic Chemistry (8) was proposed independently in 1858 by Kekulé (9a), who had just been appointed Professor at Ghent, and a young Scot, Archibald Scott Couper (1831-1892, Figure 2) (9b-d), who was a student in the Paris laboratory of Adolphe Wurtz (1817-1884) at the time. This initial version of Structural Theory was refined in 1861 (10) by the Russian, Aleksandr Mikhailovich Butlerov (Бутлеров Александр Михайлович, 1828-1886, Figure 2), an entomology graduate who had been chosen by the Curator of the Educational District for transfer into chemistry—despite little formal chemical training— to meet the needs of Kazan University. This was the second time that Kazan had been lucky: the previous non-chemist to be forced into teaching chemistry there was Nikolai Nikolaevich Zinin (Зинин Николай Николаевич, 1812-1880), a physics-mathematics graduate who was teaching hydrostatics; both Zinin and Butlerov became internationally eminent nineteenth-century organic chemists and helped to propel Kazan to the forefront of chemistry schools in Russia.

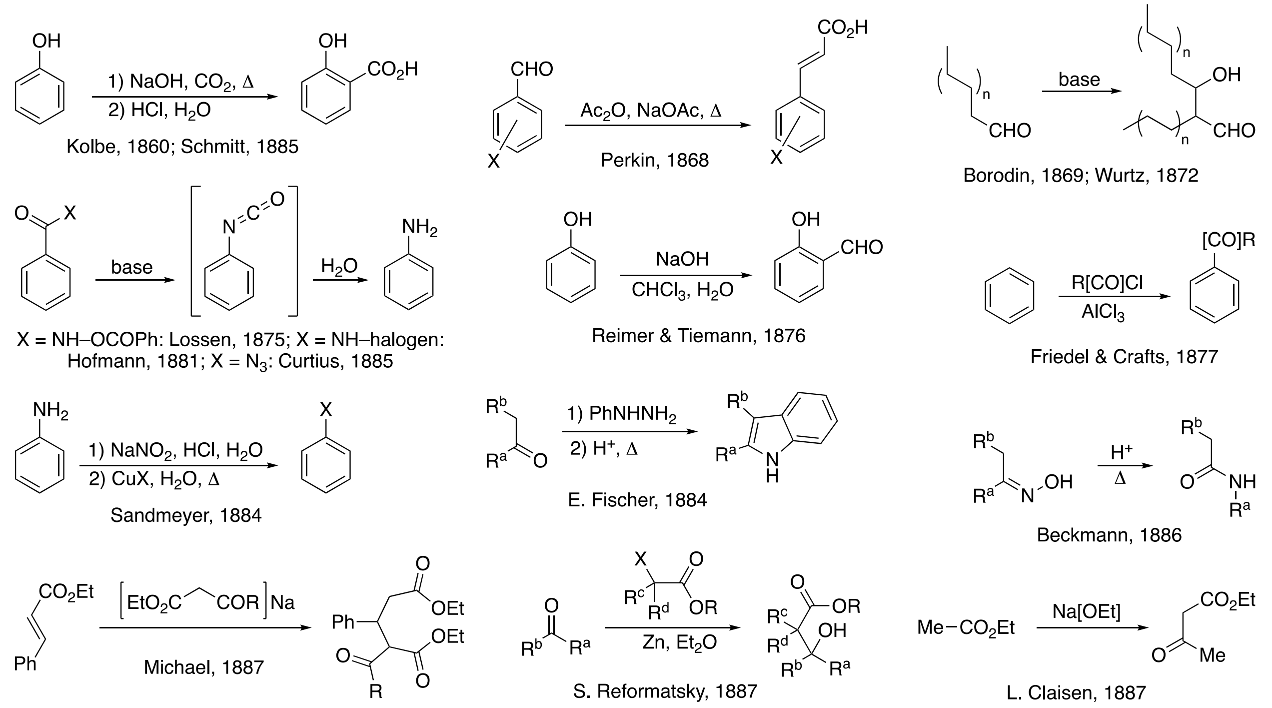
Couper Kekulé Butlerov

Figure 2. *The developers of the Structural Theory of Organic Chemistry.*

Structural Theory stimulated a wave of innovation in organic chemistry, most especially in organic synthesis. Between 1850 and 1900, over twenty well-known name reactions were discovered; representative examples from 1860-1890 are collected in Table 1. Why did this happen? And what guidance does it offer us today about where organic chemistry might go?

The answer to the first question is fairly obvious: The simple equivalent and molecular formulas that had been used since the early work of Wöhler and Liebig (11) were devoid of detail when it came to the structure of organic compounds. Now, for the first time, organic chemists had a framework that they could use to better understand the course of chemical reactions and, in the process, ask questions about how they might manipulate the reaction conditions to affect the reaction outcome.

Table 1. Representative name reactions developed between 1860 and 1890 (depicted in modern structural notation)



Organic chemistry had become a science formulated in visual, structural formulas rather than in simple molecular or empirical formulas.

The second question is more subtle, and it may well be that its answer will appear trite, but Butlerov, in particular, had shown that Structural Theory had predictive potential by predicting the structures of previously unknown alcohols *and then confirming their existence by synthesis*. This was one of the first examples of what is now a *sine qua non—today, a viable theory must have predictive potential*.

Stereochemistry

The third dimension in organic chemistry also emerged at the end of the nineteenth century (12) with the stereochemical theories of Dutch chemist Jacobus Henricus van't Hoff (1852-1911, Figure 3) (13) and French chemist Joseph-Achille Le Bel (1847-1930, Figure 3) (14), and with the discovery of his eponymous inversion reaction by Latvian chemist Paul Walden (1863-1957, Figure 3) (15).

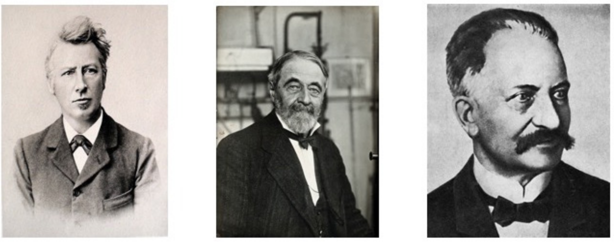
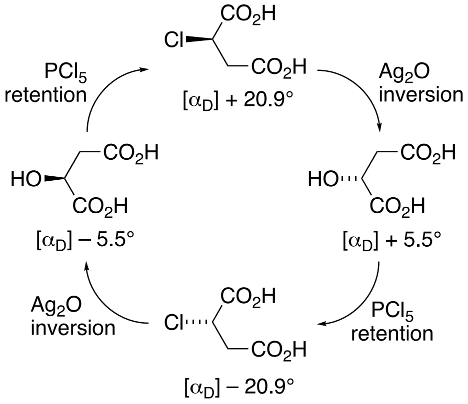

van't Hoff Le Bel Walden

***Figure 3**. Key chemists in the rise of stereochemistry*



***Scheme 2.** The Walden cycle*

Empiricism and Regiochemistry

In addition to the Name Reactions, the nineteenth century also saw the publication of empirical rules topredict reaction regiochemistry and to predict the strain in cyclic compounds (Figure 4). Prior to the emergence of Structural Theory, August Wilhelm [von] Hofmann

(1818-1892) had proposed his Rule for elimination from quaternary ammonium hydroxides (16), and had added the Ammonia Type to the dominant theory of the time, Type Theory. The search for clear experimental validation of Butlerov's version of Structural Theory drove the work of his student, Vladimir Vasil'evich Markovnikov (Markownikoff, Марковников Владимир Васильевич, 1837-1904, Figure 4), whose Rule for addition of acids to alkenes (17) emerged in 1869 as a logical offshoot of his graduate research (18). The motive for the development of the empirical rule for elimination from alkyl halides (19) by another Butlerov student, Aleksandr Mikhailovich Zaitsev (Зайцев Александр Михайлович, 1841-1910, Figure 4), was hardly altruistic: Zaitsev and Markovnikov carried on a

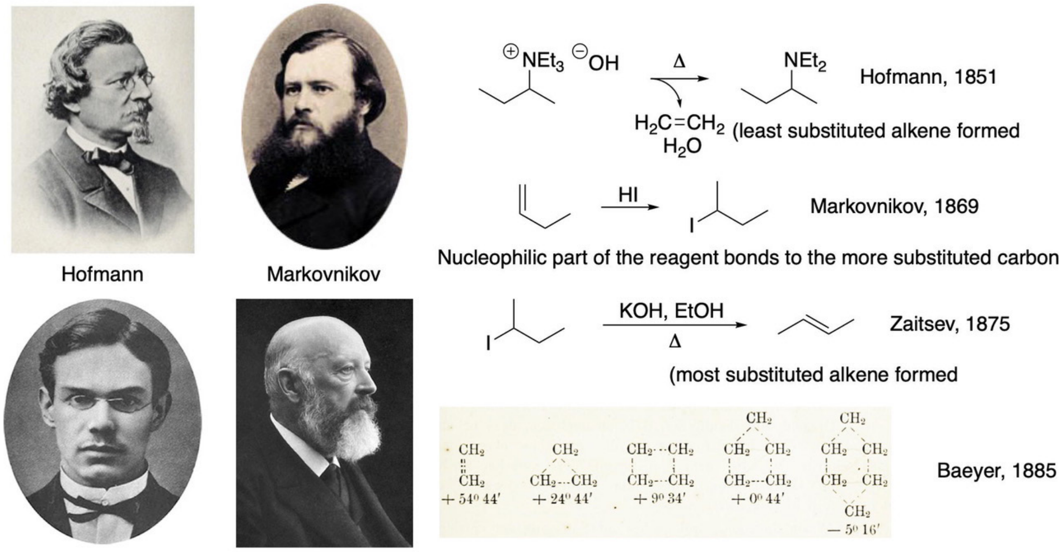


***Figure 4**. Organic chemists and their eponymous empirical rules and theories*

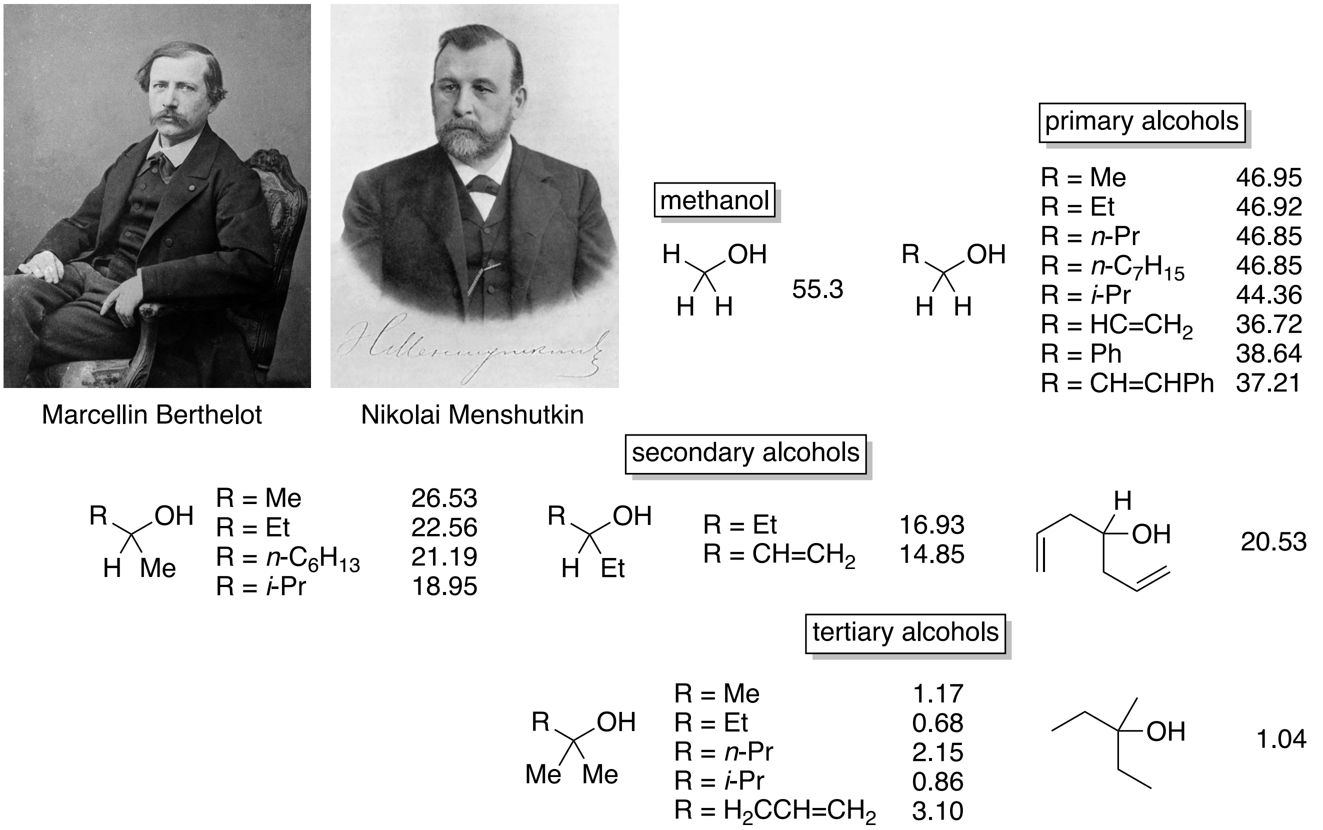


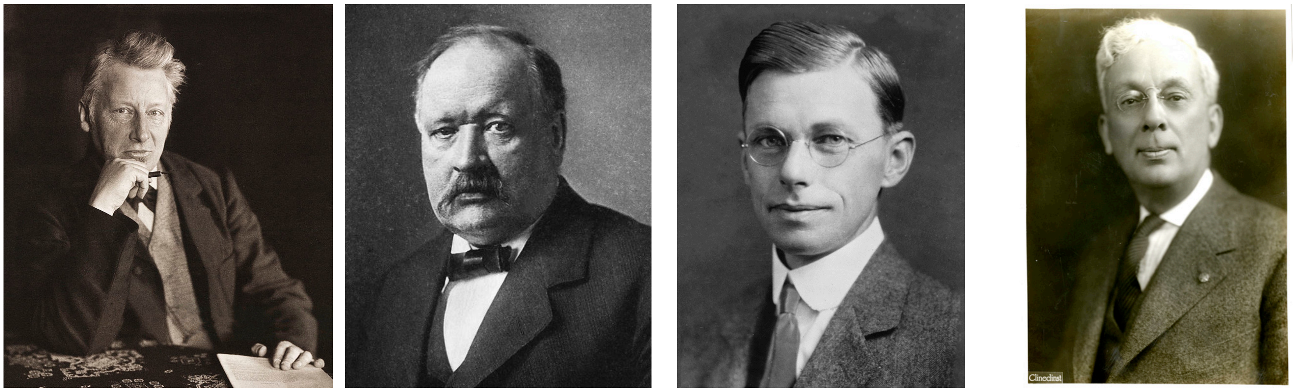
***Figure 5**. Marcelin Berthelot, Nikolai Menshutkin, and representative initial rates of acetylation of alcohols with acetic acid in a sealed tube at 155 °C as measured by Menshutkin.*

life-long feud. In 1885, Adolf von Baeyer (1835-1917, Figure 4) proposed the existence of ring strain in cyclic compounds (20). The eponymous rules and theories of these chemists are collected in Figure 4.

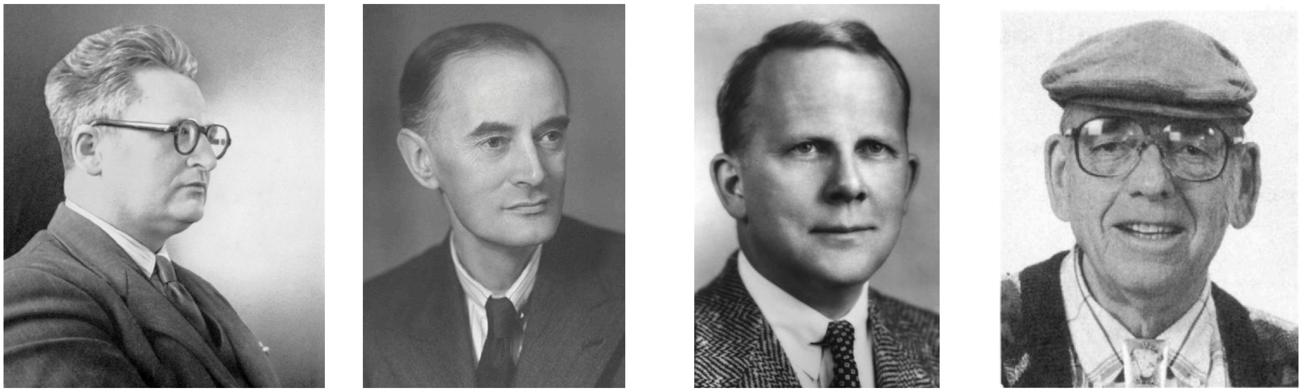
An additional question to be answered was a simple one: "What factors affect the reactivity of a functional group in an organic compound, and is the effect big enough to be exploited?" The answer to this question required answers from a new sub-discipline of organic chemistry: physical organic chemistry. The earliest work in this area consisted of rate studies of reactions. One of the first systematic reports of rate studies was disclosed in three papers between 1862 and 1863 by Pierre Eugène Marcellin Berthelot (1827-1907, Figure 5) and Léon Péan de Saint-Gilles, who were studying the rates of esterification of alcohols (21). In 1877 (22), the Russian chemist Nikolai Aleksandrovich Menshutkin (Меншуткин, Николай Александрович,1842-1907, Figure 5) began what eventually became a four decade-long study of the effects of reactant structure on the rates of organic reactions, beginning with esterification reactions (23) (Figure 5). Menshutkin followed his work on esterification by studies of the effects of amine and alkyl halide structure on the rates of alkylation of amines (24), which later became his eponymous reaction.

Following the model of Berthelot and Péan de Saint-Gilles, Menshutkin studied the initial rates of ester formation in equimolar mixtures of the alcohol and acetic acid in sealed tubes at 155 °C. These studies revealed consistent patterns of reactivity: for example, the initial rate of acetylation could be used to distinguish the alcohol as primary, secondary or tertiary.

Seven years after Menshutkin's initial studies, Jacobus Henricus van't Hoff (1852-1911, Figure 6)



J. H. van't Hoff *S. Arrhenius* *J. B. Conant* *J. F. Norris*



E. D. Hughes *C. K. Ingold* *L. P. Hammett* *R. W. Taft, Jr.*

***Figure 6**. Important early physical organic chemistsThe new evidence was provided by kinetic isotope effects (30), which gave a direct measure of bonding changes between reactants and transition state. The deuterium kinetic isotope effect, defined as $^{H}k/^{D}k$, is defined as "normal" when $^{H}k/^{D}k > 1$, "inverse" when $^{H}k/^{D}k < 1$, and "null" when $^{H}k/^{D}k = 1$. Normal isotope effects arise when the bond to the labeled atom is weakened in the transition state, and inverse isotope effects arise when the bonding to the labeled atom is strengthened. The information gleaned from isotope effect studies provided a basis for modeling transition states (30d)*

published his *Études de Dynamique chimique*, in which he first proposed his equation describing the temperature-dependence of the equilibrium constant (25).

$$\frac{d}{dT}\ln\left(K_{eq}\right) = \frac{\Delta_r H^\circ}{RT^2}$$

Five years later, Svante Arrhenius (1859-1927, Figure 6) proposed his equation relating the rate constant of a reaction and the temperature at which the reaction is carried out (26).

$$k = Ae^{\frac{-E_a}{RT}}$$

Menshutkin adopted these new approaches for his work in the 1890s and beyond.

The twentieth century saw a real blossoming of the field, with luminaries such as James Bryant Conant (1893-1978, Figure 6) and James Flack Norris (1871-1940, Figure 6), who made important contributions in the kinetics of organic reactions in the 1920s, Edward David Hughes (1906-1963, Figure 6) and Sir Christopher Kelk Ingold (1893-1970, Figure 6), and Louis Plack Hammett (1894-1987, Figure 6), whose contributions during the 1930s cemented physical organic chemistry's position as a legitimate subdiscipline of organic chemistry. The conclusions of Hughes and Ingold's sixty joint papers, collected in Ingold's monograph (27), gave us the terminology about the mechanisms of substitution and elimination reactions that is still in use today: S_N1, S_N2, E1 and E2. Hammett's simple equation (28) provided a productive springboard for the launch of modern physical organic chemistry; Robert W. Taft, Jr. (1922-1996, Figure 6), expanded the Hammett equation to include resonance and field effects (29). The work of Hammett, then Taft, shifted the focus of organic chemists to the transition state; this could not be completely successful without evidence for its possible structure.

Early Total Synthesis: Exploiting Chemoselectivity

The formal total synthesis of camphor was among the earliest successes in chemoselectivity in organic synthesis. This was accomplished by combining the conversion of α-campholide to camphor by Haller (31) with the total synthesis (32) of camphoric acid by Finnish chemist, Gustaf Komppa (1867-1949) in the form of three different reductions (Figure 7). The first, a dissolving metal reduction with sodium amalgam, reduces only the ketone carbonyl groups; the second, a Berthelot reduction (33) of the diol, leads first to hydrolysis of the diester to the diacid, which will be resistant to reduction, and then reduction to the alkene, probably through the vicinal diiodide; and the third is another dissolving metal reduction with zinc metal, which will reduce a bromide. The modern concepts of tandem or cascade reactions and biomimetic synthesis were showcased in 1917 with Robinson's classic synthesis of tropinone (34).

Diastereoselectivity in Cyclic Systems

The next major advances in organic synthesis led to the control of the relative stereochemistry of reactions. As part of this advance, the stereochemistry of organic reactions became a high-priority area of research. A

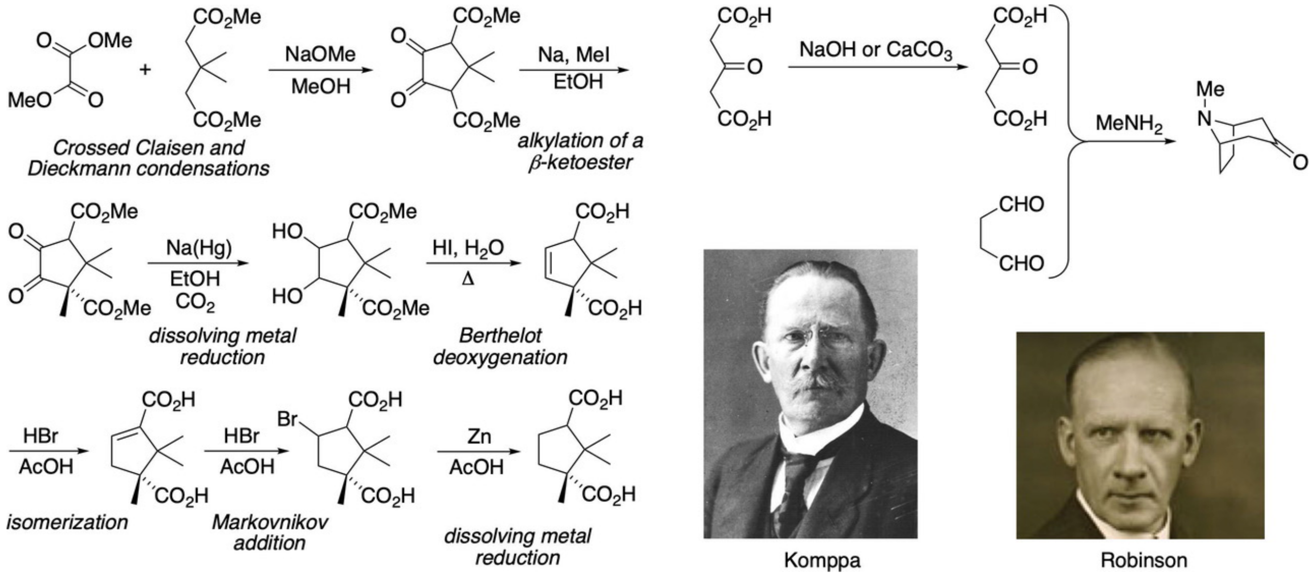
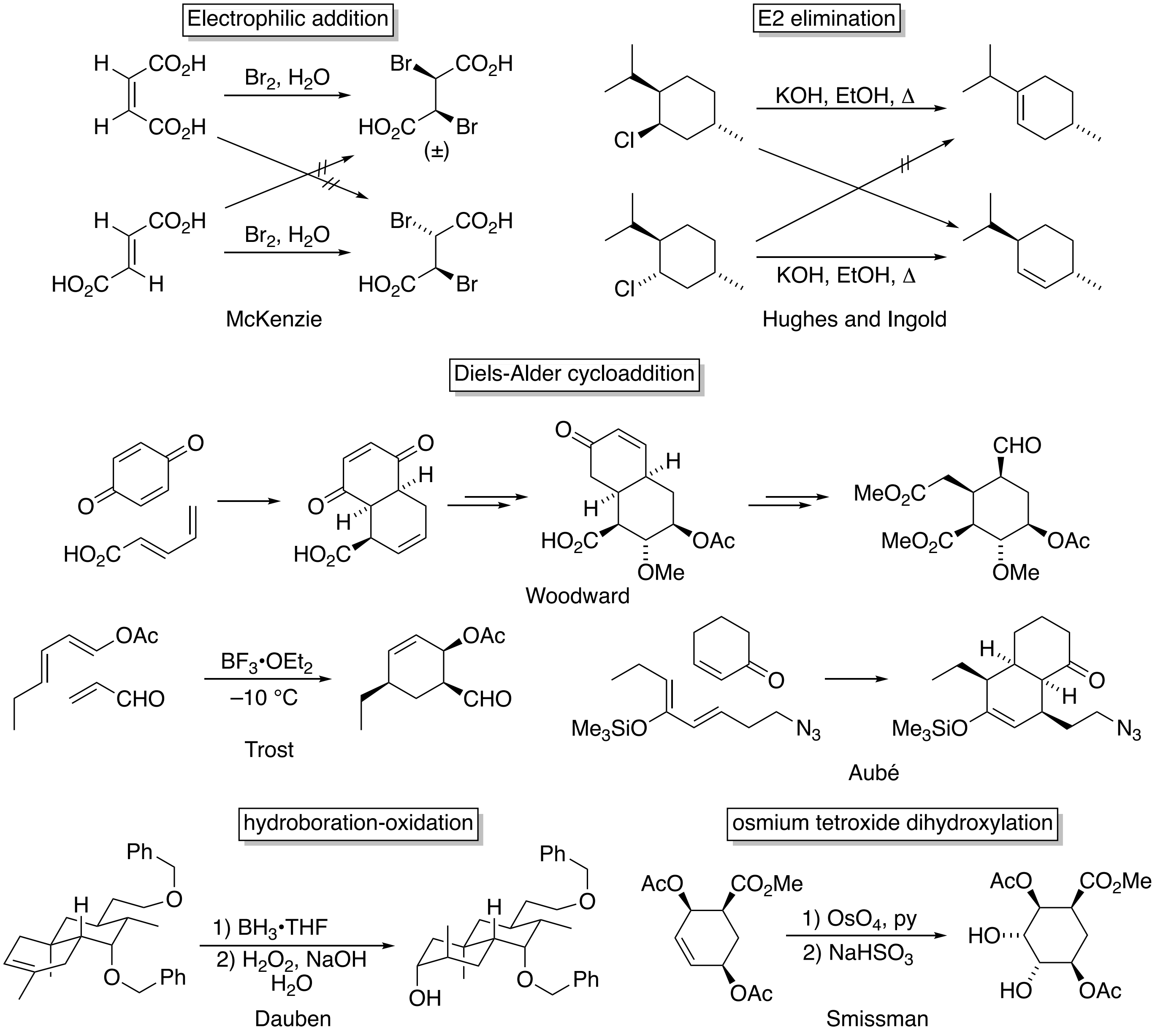


Figure *7. Komppa's total synthesis of (±)-camphoric acid, constituting a formal total synthesis of (±)-camphor, and Robinson's biomimetic synthesis of tropinone.*


Electrophilic addition

E2 elimination

Diels-Alder cycloaddition

hydroboration-oxidation

osmium tetroxide dihydroxylation

Figure 8. *Stereospecific reactions.*

collection of important stereospecific reactions is given in Figure 8.

A good example is provided by the stereochemistry of the addition of bromine to alkene π bonds. Early work by McKenzie (35) revealed that the addition of bromine to maleic acid gave *dl*-2,3-dibromosuccinic acid, and that the same reaction with fumaric acid gave the *meso* product. This result, consistent with *anti* addition to the double bond was rationalized through a three-membered bromonium ion (36). Later, Hughes and Ingold gave unequivocal evidence for the stereospecific *anti* elimination under the E2 conditions of the Zaitsev elimination (37). In 1928, one of the most valuable synthetic reactions in all of organic chemistry, the Diels-Alder cycloaddition (38), was reported by Otto Paul Herman Diels (1876-1954) and his student, Kurt Alder (1902-1958); the pair shared the Nobel Prize in 1950 for their discovery. The ability of this reaction to generate up to four new chiral centers and a cyclohexene simultaneously has made it a key synthetic method (39-41). Hydroboration-oxidation and osmium tetroxide dihydroxylation are stereospecific *syn* additions that have long been exploited for incorporating new chiral centers into a molecule (42, 43).

Acyclic Stereoselectivity

By the late 1960s, controlling the relative stereochemistry in cyclic systems had become a well-developed art. The next big hurdle was to move to acyclic systems. An early exploration of this problem by Donald James Cram (1919-2001) resulted in the empirical rule that bears his name for predicting the stereochemistry of the product of addition of a nucleophile to a chiral aldehyde (Figure 9) (44).

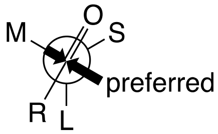


Figure 9*. Cram's empirical Rule for predicting the direction of attack of a nucleophile on a carbonyl group.*

The histories of acyclic diastereoselectivity and enantioselectivity are so intertwined that the two should be discussed together. Conformational analysis (45), for which Barton and Hassell shared the Nobel Prize for Chemistry in 1969, provided the basis for predicting the stereochemistry of transition states resulting from the preferred conformations of the reacting species. Although Cram's 1952 Rule had offered a tool for predicting the stereochemical outcomes in reactions of acyclic substrates, it took another two decades before serious efforts were made to exert stereochemical control in such systems. Why so long? It required the confluence of more advances from disparate directions before serious progress in this area could be realized:

First, methods for carrying out reactions under conditions of kinetic control needed to be developed. This paradigm shift in synthetic organic chemistry, from running reactions under thermodynamic control to running them under kinetic control, drew the attention of organic chemists to the structure and energy of the transition state for the reaction. This now highlighted the task of increasing activation energy difference between competing reactions. The solution to the problem came from the work of the early physical and physical organic chemists. Arrhenius' work, in particular, had shown that it should be possible to lower the reaction temperature to a point where even a small difference in activation energy might so retard one of two competing reactions that it would be possible to form the product of the other with a high degree of selectivity: the product of kinetic control would predominate.

Second, a vocabulary for describing the stereochemical outcome of a reaction needed to be developed. In 1971, Morrison and Mosher coined the term, "enantiomeric excess (e.e.)," in their book, *Asymmetric Organic Reactions* (46), and this term is still in use, usually as a percentage. However, in 1969 Horeau showed that the value obtained for the e.e. depends on the method used to calculate it (47), which prompted Gawley to analyze the deficiencies in the terms, "% e.e." and "% d.e.," and propose their replacement by "enantiomer ratio, er," and "diastereomer ratio, dr," instead (48).

Measuring the values of e.r. and d.r. in organic reactions also required the development of methods for doing so. Modern organic chemistry has settled on chromatography and NMR spectroscopy as the techniques of choice. The chromatographic separation of enantiomers was pioneered by William H. Pirkle at the University of Illinois in the late 1970s and early 1980s (49); the growth of the technique is illustrated by the more than 17,000 hits on the search term, "chiral chromatography," in Google Scholar since January 2020. The pioneering work of Heathcock (50) on the aldol addition reaction provided an early example of the use of NMR spectroscopy to obtain the data to assign the relative configuration to chiral centers in a molecule. Today, a combination of experimental and computational NMR methods is used to determine absolute configurations and e.r. values for reactions.

Running reactions under conditions of kinetic control required the use of cryogenic baths: dry ice-acetone (–78 °C), liquid nitrogen-ethanol (–110 °C), and liquid nitrogen (–196 °C). The manufacture of dry ice had been patented in France in May 1831 (51). An explosion in 1841 (52) served to dampen enthusiasm for its use; its use as a reaction coolant did not become routine until well into the twentieth century. The pioneering work of Heathcock, for example, could not have been accomplished without being able to access low temperatures that would suppress the isomerization of the lithium enolates. Because his work involved the correlation of product stereochemistry with reactant stereochemistry, it was imperative that the stereochemistry of the reactant not change during the course of the reaction.

Using very low reaction temperatures to moderate organic reactions also yielded another benefit: very low reaction temperatures permitted the use of extremely reactive reagents or thermally unstable reactants. Sterically hindered, strong amide bases such as lithium diisopropylamide, which can be formed by the reaction of butyllithium and diisopropylamine in tetrahydrofuran at –30 °C, have become routine reagents for forming anionic nucleophiles such as enolates, azaenolates, ylides, etc., at –78 °C.

The successes in controlling the relative stereochemistry obviously promoted interest in being able to meet the next stereochemical challenge: controlling the absolute, as well as the relative configuration of products formed from achiral precursors. The three successful strategies for accomplishing this (Figure 10) were, in chronological order: 1) chiral auxiliaries; 2) chiral reagents; and 3) chiral catalysts. All three of these approaches were based on having the reaction proceed through diastereomeric activated complexes of significantly different energy.

Where?

Chiral catalysis now falls in the mainstream of asymmetric synthesis; it is the work for which Sharpless (53), Noyori (54) and Knowles shared the Nobel Prize in Chemistry for 2001. This strategy for generating asymmetric induction, the *chiral catalyst* strategy, has taken the organic synthesis community by storm since the first reports of high levels of asymmetric induction in reactions catalyzed by metal complexes (55). The growth in the field can be gauged from the growth in size of the volumes in *Catalytic Asymmetric Organic Synthesis*, edited by Ojima (54a); the first edition (1993) had 476 pages, the second edition (2000) had 864 pages, and the third edition (2010) had 998 pages. No fourth edition has yet appeared, but it would not be unrealistic to expect that it will be more than 1500 pages. A recent search reveals that there have been 349 articles published in *Chemical Reviews* since 2008, averaging 40-50 pages per review, and a Google Scholar search on May 20, 2021, returned 3,310 hits since January 1, 2021 hits on the search term, "catalytic asymmetric synthesis."

The other area where catalysis has had a major impact has been on reaction regiochemistry. Every student of introductory organic chemistry was taught that halogens bonded to sp^2-hybridized carbon atoms are inert to displacement except under extreme conditions. That changed in 1971. That year, Tsutomo Mizoroki (1933-1980) of the Tokyo Institute of Technology reported the palladium-catalyzed cross-coupling of iodobenzene with olefins (56). These kinds of reactions, now known as cross-coupling reactions, were the basis for the Nobel Prize in Chemistry in 2010 to Heck, Negishi and Suzuki, and the related olefin metathesis reaction, for the Prize in 2005 to Chauvin, Grubbs and Schrock. A Google Scholar search using the term, "cross-coupling reactions," on May 20, 2021, returned approximately 10,000 hits since January 1, 2021. The results from searches on individual cross-coupling reactions for the same time period are gathered in Table 2.

Organocatalysis

The success of transition metal catalysts in stereoselective organic synthesis has prompted the search for efficient, metal-free catalysis of reactions (especially asymmetric reactions). Two major contributions in this area have come from the laboratories of MacMillan (57) and Shi (58), whose work first appeared around the turn

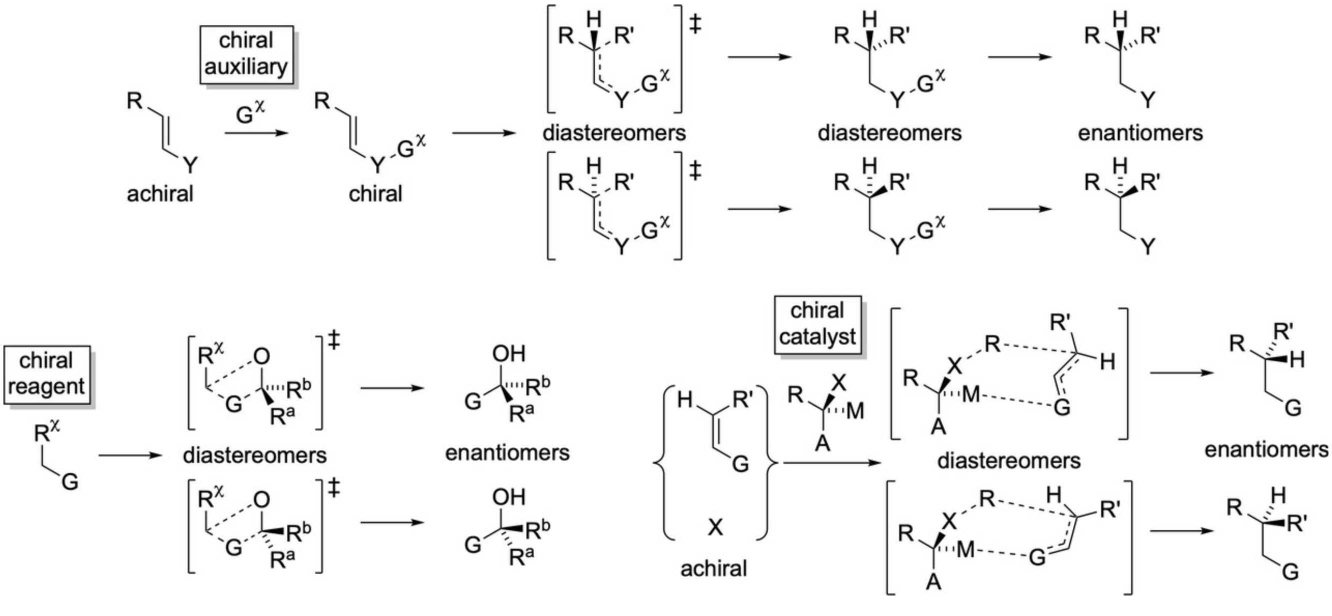


***Figure 10**. The three fundamental strategies for asymmetric synthesis. The superscript "χ" indicates that the group is a single enantiomer.*

of the twenty-first century. Indeed, MacMillan and Benjamin List were awarded the 2021 Nobel Prize in Chemistry "for the development of asymmetric organocatalysis."

MacMillan noted that iminium ions, nature's acylium ion equivalents, offer enhanced electrophilicity compared to carbonyl compounds, but do so without the recourse to strong Lewis acid catalysts, and showed that this type of electrophilic enhancement would be successful *in vitro*; his imidazolinone organocatalysts are based on proline, which itself shows modest asymmetric organocatalytic effects. By clarifying how structural changes to proline influence the efficacy of the organocatalyst, he was able to identify the key structural moieties needed to give high levels of diastereoselectivity in the transition state, and high e.r.'s in the product.

Table 2. Palladium-catalyzed Coupling Reactions Reported in 2021 (through May 20, 2021)

Reaction	Number of Hits	Reaction	Number of Hits
Suzuki-Miyaura	4,380	Heck	1,940
Sonogashira	1,380	Negishi	1,580
Olefin metathesis	1,440	Stille	1,190
Hiyama	961	Tsuji-Trost	172

The asymmetric reduction of ketones has long been problematical for organic chemists. However, the search for new chiral organocatalysts for reduction has led to the development of the oxaborolidine catalyst for the asymmetric reduction of prochiral ketones by borane derivatives, first reported by Itsuno (59) and developed by Corey (60). The oxaborolidine and the MacMillan and Shi catalysts are shown in Figure 11.

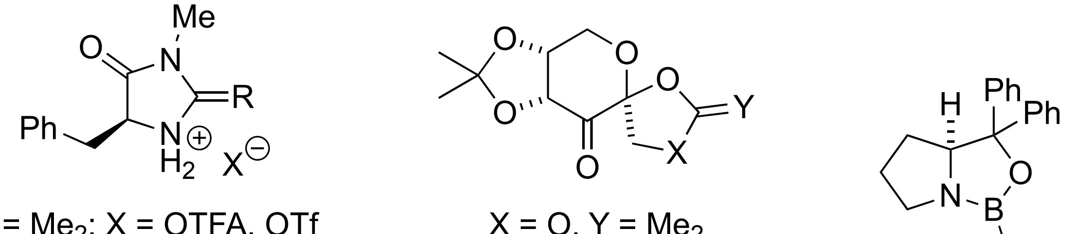
Whither?

We have now arrived at the present, so now the job is to answer the question, "whither—*quo vadimus*?" Prognostication is a perilous pastime, but since that is the basis of this Special Issue, I can but do my best. As I see it, the first question to answer is, "What lessons have we learned in the past two centuries?" The second is, "What do these lessons teach us about where organic synthesis may evolve?"

The advances in the science that have led to major improvements in being able to control selectivity in organic chemistry have not necessarily achieved contemporaneous recognition. For example, did Mikhail Tsvet and his contemporaries see the truly transformative effect of his discovery of chromatography on the course of organic chemistry? If they did, why did he receive only one nomination for the Nobel Prize? Sometimes milestones become apparent only with the passage of time—a fact that complicates the writing of recent history, let alone prognostication.

Advances in selectivity in organic chemistry have almost always correlated with progress in physical or theoretical methods. Once discovered, new techniques have diverged and specialized under the intensive research that followed, as the proliferation of chromatographic techniques shows. Thanks to advances in instrument and software design, bench-top instruments for NMR spectrometry and X-ray diffraction are now widely available; when the author was a graduate student in the 1970s, neither proposition would have been taken seriously.

Beginning with the work of Hughes, Ingold and Hammett almost a century ago, our better understanding of reaction mechanisms has allowed the outcomes of reactions to be optimized by manipulating the reaction conditions over which the chemist has control: temperature, pressure, solvent, reagent power and concentration.



R = Me_2; X = OTFA, OTf
R = H, t-Bu, Ar; X = OTFA, OTf
MacMillan imidazolinones

X = O, Y = Me_2
X = N–Ar, Y = O
Shi ketones

Corey oxaborolidine

Figure 11. *Chiral organocatalysts*

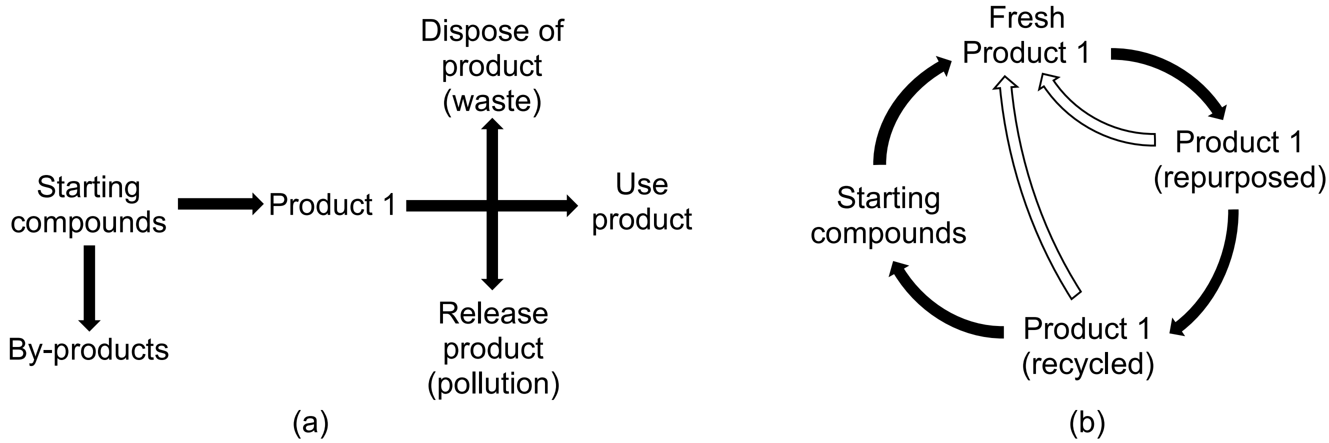


***Figure 12**. The linear (a) and cyclic (b) views of the progression from raw materials through organic chemistry.*

One can select for the S_N1 reaction, for example, by using a low concentration of a weak nucleophile in a protic solvent. In the 1950s, conformational analysis was developed, giving the organic chemist a way to "see" the dynamic shapes of molecules. By using these concepts, organic chemists were able to design stereocontrolled total syntheses of complex natural products.

Today, computational chemistry is being used to reveal the basis for empirical rules that have long been a mainstay of organic chemistry—Hofmann's Rule for elimination (16), Markovnikov's Rule for addition (17, 18) and Zaitsev's Rule for elimination (19). For example, the origins of Markovnikov regioselectivity (61) are being elucidated *in silico*.

Until the last decades of the twentieth century, useful, stereoselective catalytic organic reactions were few and far between. That changed with the Sharpless asymmetric epoxidation (53). For the first time, it was possible to prepare a chiral product from a prochiral starting compound and an achiral reagent with known absolute configuration and high e.r.'s and d.r.'s, an accomplishment previously limited to enzymes. Reactions catalyzed by transition metal complexes have made asymmetric syntheses that would not have been seriously contemplated half a century ago, fairly routine. At the same time, these reactions have also turned the conventional wisdom on its head: the categorical statement, that nucleophilic displacement of leaving groups from sp^2-hybridized centers other than acyl groups is not easy to accomplish, is contradicted by reactions such as the Heck, Stille, Suzuki and Sonagashira cross-coupling reactions. The difficulties inherent in the synthesis of macrocyclic compounds have been circumvented by olefin metathesis.

So, once again, "whither?" I believe that Green Chemistry will have a major impact on organic chemistry, an opinion shred by Javier Garcia-Martinez, Vice-Chair of the Bureau of IUPAC (62). This vision sees the organic synthesis enterprise moving from the traditional linear progression through organic chemistry, where the trajectory is unidirectional, from starting materials through to the target product and waste; as we know, much of the final product ends up as waste, also. The alternative progression through the same lifespan is dramatically different. In the idealized system in Figure 12, there is no waste, but the starting material is cycled through useful products until it reaches the end of its useful lifetime, whereupon it is reconverted to the starting compounds, which are then used to re-form the original product. As drawn, this cyclic system has no losses or waste, but today that is still an unattainable, though not unworthy goal.

How does the history of organic chemistry provide a blueprint for how we move forward? It took the combined efforts—often not in intentional collaboration—of synthetic organic chemists, whose efforts added to the library of synthetic methods, physical organic chemists, whose efforts elucidated the detailed mechanisms of reactions, and analytical chemists and spectroscopists, who developed the techniques for separation, purification, and structure elucidation of organic compounds (again, often not recognized as paradigm-changing at the time) to get us to where we are now, and it is not unreasonable to expect that the next major advance may already occurred, but may not yet have been appreciated. Increased collaboration between different subdisciplines, which we are already seeing to a higher degree than heretofore, will, in my opinion, be the most important circumstance allowing us to achieve the goal.

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THE DEVELOPMENT OF MEDICINAL CHEMISTRY AS A DISCIPLINE: A TOPIC RIPE FOR HISTORICAL EXPLORATION

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Abstract

Although there has been a substantial amount of research and publication related to the history of the chemistry of drugs, there is a dearth of literature on the institutional and disciplinary history of medicinal chemistry. Medicinal chemistry did not become a recognized, distinct sub-field of chemistry until the twentieth century. This paper will discuss the opportunities for historians of chemistry and pharmacy in the exploration of the subject. It will delineate some of the interesting historical questions and themes and suggest possible sources and approaches that might lead to fruitful research in this area.

Although interest in the chemical aspects of drugs goes back at least to Paracelsus and the iatrochemists, it was only with the emergence of chemistry, especially organic chemistry, and pharmacology as distinct disciplines in the nineteenth century that significant progress was made in the isolation and synthesis of pure chemicals with physiological activity. And it was only in the twentieth century that significant progress was made in understanding the chemical interactions with cells that produced the specific effects of drugs. Especially important was the work of the German physician Paul Ehrlich in the early years of the century which led to the development of the receptor theory of drug action and the field of chemotherapy. Although there were some attempts to relate chemical structure to pharmacological action in the nineteenth century, it was Ehrlich who systematized and popularized this approach (1).

These advances led to the emergence of a group of chemists who focused their attention on the chemistry of drugs, founding the field of medicinal chemistry. What exactly is medicinal chemistry? In 2017, Selina Holbrook and Sylvie Garneau-Tsodikova addressed this question in *MedChemComm*. They wrote (2):

> This question still puzzles even the most experienced researchers working in this scientific discipline and generates a lot of discussion amongst those entering as well as those mature in the profession.

Andrew Coop, in the latest edition of the influential *Foye's Principle of Medicinal Chemistry*, addresses the problem of defining medicinal chemistry as follows (3):

> Medicinal chemistry has as many definitions as those doing the defining, and is complicated by the concurrent use of terms such as pharmaceutical chemistry, drug chemistry, bioorganic chemistry, chemical biology, and the list goes on.

He himself offers the very broad and somewhat vague definition of the subject as "the application of chemistry to the continuous improvement of health."

A particular complication, referred to by Coop, is that the term pharmaceutical chemistry is frequently used to refer to the same types of activities that define medicinal chemistry. A search of the literature shows that sometimes the terms medicinal chemistry and pharmaceutical chemistry are used synonymously and sometimes they are given somewhat different definitions. It is also not uncommon to find one of them described as a sub-field of the other, with either one of them considered the broader term. For my present purposes, I will include both in my analysis, distinguishing between them only when it seems appropriate. Medicinal chemistry should also not be confused with medical chemistry, the teaching of chemistry in medical schools, which was focused more broadly on the chemical aspects of medicine in general. Medical chemistry, as Robert Kohler has shown, eventually evolved into physiological chemistry and biochemistry (4).

There is thus no one generally agreed upon definition of the field, although I believe that there is a general understanding of what medicinal chemistry involves. For my purpose here, I will use the description of what medicinal chemists do provided by the American Chemical Society on its website page on careers in the field, which I think incorporates at least most of the activities included in typical definitions of the field (5).

> Medicinal chemists apply their chemistry training to the process of synthesizing new pharmaceuticals. They also improve the processes by which existing pharmaceuticals are made.
>
> …
>
> Medicinal chemists are focused on drug discovery and development and are concerned with the isolation of medicinal agents found in plants, as well as the creation of new synthetic drug compound.

Medicinal or pharmaceutical chemistry seems to have become a recognized, distinct division or subdivision of chemistry in the twentieth century. Historians of chemistry, medicine and pharmacy, especially over the past couple of decades, have devoted substantial attention to the history of the isolation, synthesis and uses of drugs. There have also been studies of the history of structure-activity relationships, receptor theory, and drug development. However, almost no work on the institutional and disciplinary history of medicinal chemistry has been published. The purpose of this essay is to encourage the investigation of this subject by delineating interesting historical questions and themes and suggesting possible sources and approaches that might lead to fruitful research. Given the limited space available to me, I will limit my scope to the development of medicinal chemistry in the United States.

The history of medicinal chemistry must be viewed within the broader context of the history of disciplines in general. Historian Suzanne Marchand pointed out in an essay in 2014 that the history of disciplines essentially emerged as a serious area of study in the late 1950s and early 1960s. She further argued that it was "practiced chiefly by North American scholars, and especially by intellectual historians and historians of science." Marchand expressed the view that the 1980s and 1990s represented the heyday of the history of disciplines, and that the field "has had its day" (6). Even if the history of disciplines is now in eclipse, as Marchand argues, there is still significant interest in the subject and I believe that this approach remains fruitful, especially with regard to fields whose disciplinary history has not been adequately examined.

An edited volume of essays published in 1972 outlined some of the issues involved in the history of scientific disciplines and discussed the development of a number of fields. The introduction in the book, titled "Problems in the Emergence of New Disciplines," provided examples of some of the general questions that scholars should be investigating. To paraphrase just a few of these questions (7):

1. Did research in the emerging discipline originate and spread within universities or other institutions?

2. Were other changes occurring within the social context (economic, political, etc.) in this period that were especially favorable or unfavorable to the exploration of the field?

3. To what extent did the introduction of technical information generated outside the research community of the new field affect scientific developments within the discipline?

This volume included case studies of two areas of chemistry, physical chemistry and agricultural chemistry (8). In his 1990 book, *Physical Chemistry from Ostwald to Pauling: The Making of a Science in America*, John Servos traced, as the subtitle implies, the emergence and growth of the discipline in the United States (9). Robert Kohler traced the development of a discipline closer to medicinal chemistry in *From Medical Chemistry to Biochemistry: The Making of a Biomedical Discipline* (1982) (4). Just recently, in 2020, Jeffrey Seeman and Guillermo Restrepo used an analysis of changes over the decades within the Nobel Prize in Chemistry program to present a convincing argument that biochemistry has evolved into a distinct discipline from chemistry (10).

These studies provide models for the type of disciplinary history of medicinal chemistry that I am proposing. I am not concerned with the question of whether medicinal chemistry is truly a distinct discipline from chemistry itself. It might be more properly viewed as a subdiscipline, but the issues involved in tracing the history of the field are the same. I am aware of only one book devoted to the history of medicinal chemistry, William Remers' *A History of Medicinal Chemistry* (2011). While this work provides a useful and wide-ranging account of the subject, it is confined largely to chronicling the history of the development of theories, techniques and compounds, and says little about the institutional history of the discipline. Nevertheless, it is an essential reference tool. In his book, Remers clearly points out some of the complications involved in telling the story of "how medicinal chemistry fits into the formal structure of academic and research institutions," adding that "this picture is rather confusing." He goes on to correctly indicate that the "only recognized medicinal chemistry departments in American universities are located in pharmacy colleges," and that even here they may be called either medicinal chemistry or pharmaceutical chemistry. In some cases, medicinal chemistry may be merged with pharmacology or natural products chemistry into a single department (11).

Although there are few if any organized divisions of medicinal chemistry in chemistry departments, as Remers also points out, this does not mean that individuals who identify as medicinal chemists do not exist in such departments, although they may be part of a broader organic chemistry group. The presence of many key contributors to the field in chemistry departments is shown, for example, by the number of recipients of awards given by ACS Division of Medical Chemistry to individuals in these departments (12). These chemists played an important role in the development of medicinal chemistry as a discipline. For example, Alfred Burger of the University of Virginia's Department of Chemistry founded the *Journal of Medicinal and Pharmaceutical Chemistry* (now the *Journal of Medicinal Chemistry*). Although there are some medicinal chemists located in medical schools, these schools in general do not have separate departments or units of medicinal chemistry, and medicinal chemists housed in them appear to represent only a small proportion of practitioners in the field. Of course, medicinal chemists also work in non-academic institutions, most notably in pharmaceutical companies and government research laboratories.

Perhaps the earliest sign that medicinal or pharmaceutical chemistry was becoming a distinct discipline in the United States was the creation of the Division of Pharmaceutical Chemistry of the American Chemical Society in 1909. It evolved out of a special interest subgroup known as the pharmaceutical section. Most of its early members were pharmacists who were largely concerned with plant products, drug formulation and assay methods. The advent of World War I led to a change in focus. Up to that time, the United States had been almost exclusively dependent upon Germany for the importation of synthetic drugs and intermediates, but the British blockade cut off these supplies. It became necessary for the American pharmaceutical industry to produce such products and for American chemists to undertake research on drug development and synthesis. The industry exploded in the post-war period (13). A growing interest in the chemical structure of drugs and its relationship to biological activity, as well as in drug synthesis, led the Division to change its name in 1920 to the Division of Medicinal Products and again in 1928 to the Division of Medicinal Chemistry.

It was in the period following World War II that the discipline really began to flourish. The American pharmaceutical industry became a world leader in drug research, opening up many more positions for medicinal chemists. Chemistry departments developed programs to train such individuals, as did pharmacy schools, which had become much more science-based and involved in graduate education, with many establishing departments of medicinal chemistry. The first American journal in the field was founded in 1959 as the *Journal of Medicinal and Pharmaceutical Chemistry*, dropping the *Pharmaceutical* in 1963. These were all signs indicating that medicinal chemistry had become an established discipline (14).

This brief and superficial overview of the evolution of the field in the United States suggests some obvious topics for historical investigation. For example, we need to know much more about the founding of the ACS Division of Pharmaceutical Chemistry and its transformation into the Division of Medicinal Chemistry. What forces led the founders to create a special interest group and then press for it to attain Division status? Who were the individuals responsible for the change of focus of the Division from largely pharmaceutical concerns to chemical ones, and how did they bring about this change? When did members of the division begin to think of themselves specifically as medicinal chemists? How did the Division change over time? What role did it play in the development of graduate programs and publications in the field? How did the content of articles in the *Journal of Medicinal Chemistr*y differ from the content of articles in related journals such as the *Journal of Organic Chemistry*?

Other important topics in need of research include the development of teaching and graduate programs in medicinal chemistry in departments of chemistry and schools of pharmacy and the institutionalization of research in the field in academia, the pharmaceutical industry and government laboratories. When, where and why did these developments take place, and who were the key figures involved? How did medicinal chemistry differ in each of these environments? What problems did medicinal chemists face in establishing the subject as a recognized discipline? What were the backgrounds of persons entering the field, especially in the early period when there were no graduate programs devoted specifically to medicinal chemistry?

In order for someone to develop a synthetic history of the field, there needs to be much more research on these types of questions. In addition, we need biographical studies of key individuals in the discipline and institutional histories of academic, industrial and government programs in medicinal chemistry. Work is also needed on the relationships between medicinal chemists in these different settings. John Swann's book on *Academic Scientists and the Pharmaceutical Industry. Cooperative Research in Twentieth-Century America* (1988) provides an excellent starting point for future research in this area (*15*). The history of medicinal chemistry must also be studied in relationship to related disciplines, such as organic chemistry, biochemistry and pharmacology.

There is relatively little in the historical literature addressing the types of questions raised above. For example, two histories of ACS and Remers' book devote less than a page each to the founding of the Division of Pharmaceutical Chemistry and its change of name and focus (16). A useful starting point for researching the history of the Division is Patrick Woster's article in the *Journal of Medicinal Chemistry* on the occasion of the Division's centennial in 2009. Woster has also written an article chronicling the history of *Annual Reports in Medicinal Chemistry* from its founding in 1965 up to 2015 (17). Such organizations and publications played a crucial part in the development of the discipline of medicinal chemistry.

What are some of the primary sources that historians can draw upon to tell this story? Obviously, archival and manuscript collections of individuals and institutions are a major resource crucial to the research of historians in any field. There is no specific guide to archival and manuscript collections in the history of medicinal chemistry. The Center for the History of Chemistry (now the Science History Center) published a guide to archival and manuscript collections in chemistry and chemical technology in 1987, and, although dated, it has some limited use in identifying collections related to medicinal chemistry. The publication's index, however, lists only three collections under the heading of pharmaceutical chemistry and there is no entry for medicinal chemistry. However, there may be relevant materials in collections indexed under headings such as organic chemistry and the pharmaceutical industry (18).

Ideally, historians would be able to consult the archival records (correspondence, minutes, etc.) of key institutions such as the Division of Medicinal Chemistry. My searches of the literature and contacts with the Division itself, however, have not turned up any substantial cache of historical records for the Division. There might be a limited amount of useful material in the five boxes of Records of the American Chemical Society Committee on Divisional Activities in the Othmer Library of Chemical History at the Science History Institute in Philadelphia (https://www.sciencehistory.org/othmer-library). This committee is responsible for the oversight and coordination of the activities of the various divisions, and the Division of Medicinal Chemistry is among those represented. The catalog record, however, indicates that the bulk of this collection dates from the period 1960-1982, so there would appear to be little material relating to the early decades of the Division. The Othmer Library also contains records from several of the ACS Divisions, but the Division of Medicinal Chemistry is not among them, and it is possible that no significant archives for the Division exist. Unfortunately, I have also not been able to locate an archive of historical records for the *Journal of Medicinal Chemistry* in my search of the literature and contacts with the editors of the publication.

It would be instructive to understand the development of interest and expertise in medicinal chemistry in the pharmaceutical industry, and large American firms such as Eli Lilly and Merck do maintain archival collections. I used some of these materials many years ago in the research for my book on the history of American pharmacology (19). In my discussions with other historians in more recent times, however, I have learned that it has become increasingly more difficult to obtain access to these company archives. These archives represent a potentially rich source of information on the history of medicinal chemistry within the commercial sphere, and I encourage historians to continue to make efforts to gain access to them. The personal papers of scientists who worked in industry (see examples below) can be another source of relevant information.

For those interested in the development of the field within the federal government, the voluminous records at the National Archives and Records Administration

(NARA) are a potential resource, especially the records of agencies such as the National Institutes of Health (NIH) and the Food and Drug Administration. Searching NARA's catalog on its website (https://www.archives.gov) is the logical place to start, but there is a large amount of material and it is not generally described in enough detail to make it easy to focus in on the desired items. One first needs to research the history of these agencies to identify which of their divisions/units were the principal homes for medicinal chemists and their work. Examples of areas where medicinal chemists have worked at NIH are the Division (later Laboratory) of Chemistry, now incorporated into the Laboratory of Bioorganic Chemistry of the National Institute of Diabetes and Digestive and Kidney Diseases, the Unit of Chemotherapy established during World War II (which concentrated on antimalarial drugs), research programs on drug addiction (which were eventually incorporated into the National Institute on Drug Abuse), and cancer chemotherapy programs within the National Cancer Institute (20). It would also be profitable to look at the funding of research in medicinal chemistry by government agencies such as NIH to shed light on changes in research trends in the field. When delving into any of these types of records, it is advisable to consult with an archivist at NARA before planning a visit.

Tracing the development of medicinal chemistry in academia is another important part of the story, and this occurred, as mentioned above, largely in departments of chemistry and schools of pharmacy. University catalogs are a useful resource for tracing the evolution of courses and graduate programs in medicinal chemistry. In the case of pharmacy, it is fortunate that there is a large collection of school of pharmacy catalogs in the Kremers Reference Files (https://aihp.org/collections/kremers-reference-files/) of the American Institute of the History of Pharmacy (AIHP) at the University of Wisconsin-Madison. The collection consists of catalogs from well over a hundred schools of pharmacy, some now defunct, from some 40 states, as well as a number of catalogs from foreign schools. A list of the catalog holdings is available from the AIHP (contact aihp@aihp.org). This resource would be valuable for understanding the development of medicinal chemistry in American schools of pharmacy.

Chemistry departments do not generally issue separate catalogs of their programs, so information on medicinal chemistry in these departments would have to be gleaned from more general university or college catalogs. I am not aware of any single significant collection of catalogs from different universities, and relatively few such catalogs appear to be available online in digital form. Researchers would have to consult these documents in individual university libraries and archives. In addition to the catalogs, an important source for investigating the development of medicinal chemistry graduate programs in chemistry departments is the ACS Directory of Graduate Research, issued biennially from 1953. This publication, which eventually evolved into an online version (DGRweb) was discontinued in 2016. Unfortunately, the online database is no longer available. The Othmer Library, however, has print copies of the majority of the directories issued between 1955 and 1979.

The records of pharmacy schools and chemistry departments housed in university archives are another resource for tracing the development of the field in academia. Most major university archives have online catalogs that would assist historians in identifying these sources. Historians could narrow this task of selecting which pharmacy schools and chemistry departments to focus on by using secondary sources on the history of medicinal chemistry and other published works to identify institutions that have played an obviously significant role in the development of medicinal chemistry in this country. Identifying key academic leaders in the field, as discussed below, could also assist in deciding where to concentrate one's efforts.

Published histories of schools of pharmacy, departments of chemistry and universities can also provide information on the development of medicinal chemistry and help identify the most influential departments in advancing the field in academic institutions in the United States. A good place to start in identifying histories of schools and colleges of pharmacy is the section on "Education" in *The History of Pharmacy: A Selected Annotated Bibliography* (21). There are published histories of the medicinal chemistry departments at the Colleges of Pharmacy of the University of Minnesota and Ohio State University, the only ones of their kind that I know of (22). A relatively few histories of departments of chemistry, such as those of the universities of Wisconsin, Tennessee and Arizona, have been published and these may be a source of relevant information (23). Histories of many major universities also exist, although these are not likely to provide much information specifically on medicinal chemistry programs.

Another potential resource for researching the evolution of medicinal chemistry in the United States is the personal papers of practitioners of the discipline. In addition to providing information on the careers of these individuals, these records could also shed light on relevant developments within the institutions in which they worked and the professional organizations with which they were affiliated. Sources for identifying key individuals who influenced the discipline include the lists of award winners (12) and the Hall of Fame of the ACS Division of Medicinal Chemistry (24), available on the Division's website (https://www.acsmedchem.org/), and a list of the Chairs of the Division through 1976 in a book on the history of ACS (25). Obituaries and biographical and autobiographical sketches can also serve as starting points for research in this area. A number of useful autobiographical essays by medicinal chemists can be found in the pages of *Annual Reports in Medicinal Chemistry* and *Medicinal Chemistry Reviews*.

For academic chemists, any surviving papers will often be housed in the archival collections of the universities with which they were most closely identified. For example, the papers of Sidney Riegelman, a pharmaceutical chemist who was a pioneer in pharmacokinetics and biopharmaceutics, are in the University of California, San Francisco Archives (26). The Othmer Library also houses several collections of papers of prominent medicinal chemists, including some who worked in the pharmaceutical industry such as Max Tishler and Lloyd Conover.

Oral histories of medicinal chemists can also be a valuable source of information. The Center for Oral History at the Science History Institute (27) includes in its collection interviews with a number of individuals who have worked in the field of pharmaceutical and medicinal chemistry, such as Ernest Volwiler and Paul Anderson. Transcripts of the interviews are available for consultation at the Institute or copies may be ordered from the Center for Oral History. Although the earliest pioneers of medicinal chemistry are now deceased, the fact that the field has developed significantly in the past half a century means that many important figures who have helped shape the discipline are still living. This provides historians with an opportunity to conduct oral histories with these chemists to preserve their recollections and insights, although time is of the essence here because many of them are advanced in years. A couple of examples of those who should be interviewed are Philip Portoghese, Editor-in-Chief of the *Journal of Medicinal Chemistry* from 1972 to 2011, and Kenner Rice, longtime Chief of the Drug Design and Synthesis Section of the National Institute on Drug Abuse.

Lastly, I would cite as another source of potential information on the history of medicinal chemistry databases such as SciFinder and Web of Science. For example, one can use them to track the number of papers published in medicinal chemistry by years or decades in order to chart the growth of the field. I have utilized this technique myself in other contexts using Science Citation Index (included in Web of Science). Citation indexes can also be used in the tracing of networks of researchers in the field.

I hope that this brief survey of issues and sources related to the history of medicinal chemistry as a discipline will serve to stimulate further research on the subject. Studies on the science of medicinal chemistry (e.g., theories, drug discovery) will and should continue, but these must be complemented by research on the development of the subject as a distinct discipline in order to paint a more complete picture of the history of the field. The histories of the science and discipline of medicinal chemistry are of course not totally separate fields. Each influences the other and both are needed for a comprehensive picture. To give just one example, how has the life of a medicinal chemist changed over the past century with respect to such factors as areas and methods of research, types of institution worked at, sources of research support, and perception of the field by participants and outsiders? Obviously both scientific and institutional factors have influenced changes in what it means to be a medicinal chemist.

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About the Author

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MOVING BEYOND THE INTERSECTION OF CHEMISTRY AND HISTORY: EVOLVING MULTIDISCIPLINARY APPROACHES TO THE HISTORICAL STUDY OF CHEMISTRY

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Abstract

The increasing frequency of multidisciplinary research in science has largely resulted from an effort to address increasingly complex problems, particularly in the realms of medicine, the environment, and materials science. While the focus of multidisciplinary research has been on the sciences, there is a growing call to apply multidisciplinary approaches to the humanities as well. While such calls are largely concentrated on applications to education in the humanities, it is a simple extension to consider such approaches to humanities research as well. It is with such a view that the current report provides a discussion of the evolving multidisciplinary approaches to the study of history, with particular focus on the history of chemistry.

Introduction

The descriptor *multidisciplinary* has become so ingrained into the scientific endeavor that it becomes yet another common buzzword to which we rarely give further consideration. Still, the reality is that it has developed into a critical aspect of modern science and probably deserves more focused attention. According to Merriam-Webster, multidisciplinary is defined as "combining or involving more than one discipline or field of study" and is synonymous with the descriptor *interdisciplinary*. Others, however, have attempted to distinguish between the related terms multidisciplinary and interdisciplinary based on the level of integration of the different disciplines involved (1, 2). In such discussions, multidisciplinary is specified as the application of different disciplinary perspectives to a common topic, but without significant integration of those perspectives. In contrast, interdisciplinary is used to describe the more integrated approach in which disciplines are combined to result in new theoretical, conceptual, and methodological frameworks. At the same time, it has also been pointed out that such distinctions lead to confusion and are not always very practical as this attempts to assign a level of precision not always present and thus risks missing the essential nature of multidisciplinary/interdisciplinary activities (2, 3). Here, we will limit ourselves to the more general view of multidisciplinary, without any specific concerns about the level of integration between the various disciplines.

The increasing frequency of multidisciplinary research in science has largely resulted from an effort to address increasingly complex problems (2, 4-7), particularly in the realms of medicine, the environment, and materials science. Of course, such interdisciplinary research either requires an individual researcher to gain a depth of understanding in two or more disciplines, including some fluency in their terminologies and methods, or the assembly of multidisciplinary teams to work together on a specific problem (6). It is this second approach that is more frequently applied (2, 6, 7). Regardless of the specific path taken, however, such multidisciplinary approaches have successfully fostered new lines of thought and the emergence of new formal disciplines (5). This can be due to the existence of large knowledge gaps between disciplines or even between specializations within disciplines, requiring the need for additional bridging fields (2).

Evidence has also been presented that crossing disciplinary boundaries leads to increased creativity and helps to foster innovation (5-7). Furthermore, it has been found that multidisciplinary efforts appear to have a stronger connection to innovation than the number of countries involved in international collaborations (5). At least some of this is attributed to the view that ideas and methods are most often transformational when drawn from outside the discipline that developed them (6). A commonly cited example of this was the discovery of X-rays by the German physicist Wilhelm Röntgen (1845-1923) in 1895 (8). Although Röntgen produced the first X-ray image and recognized its potential applications, it was later experimentation by medical practitioners that made the modern X-ray image a game-changing medical tool. As such innovation can in turn lead to job creation, economic growth, and increased competitiveness (5), multidisciplinary efforts have become increasingly favored by both industry and government (2).

While the focus of multidisciplinary research has been on the sciences, there is a growing call to apply multidisciplinary approaches to the humanities as well (9-11). While the focus for such calls is primarily on education in the humanities, it is a simple extension to consider such approaches to humanities research as well. It is with such a view that the current report will provide a discussion of the evolving multidisciplinary approaches to the study of history, with particular focus on the history of chemistry.

Traditional Multidisciplinary Aspects of Historical Studies

While the most traditional approaches to the study of history have been the analysis of primary and secondary sources, historians have long borrowed from, overlapped with, and incorporated other disciplines, particularly those of archaeology, linguistics, and statistics (12). While the goal is not to provide a comprehensive discussion of such traditional methods, it is worth presenting a brief discussion of a few examples.

Perhaps the most obvious and long-standing overlap is between that of history and archaeology. The use of archaeology as a critical tool by historians dates back to the 18th century, largely driven by the discoveries of Pompeii and Herculaneum in 1748 and 1738, respectively (12). Archaeological evidence is, of course, most precious for lost civilizations, and is sometimes the only way to obtain knowledge about such histories. This is especially critical for time periods that predate written records, with the bulk of human history providing only material evidence until ca. 5000 years ago (12). In terms of the history of chemical practice, this applies directly to various early chemical technologies, including pigments and dyes, pottery and ceramics, fermented beverages, metals, and glass (13-15).

Another classical example of traditional overlap between disciplines in the study of history is the application of historical linguistics, with particular focus on etymology (the study of the origin and uses of words) and historical semantics (study of the changing meanings of words through time) (12, 16, 17). The history of chemistry has a number of notable cases in which knowledge of the origin and changing meaning of key terms is integral to understanding the underlying history. Perhaps the most colorful example of this would be the word *alcohol*, which finds its origins in *kohl* (or *kuhl*), the name of a mineral cosmetic from antiquity (18-20). During the rise of the Islamic Empire in 7th century, the word was then modified with the Arabic prefix *al-* to become *al-kohl* (or *alkuhl*), while still retaining its original meaning. Over time, however, the meaning of the word did undergo gradual change to ultimately refer to first ethanol in the 16th century and later the general chemical class of alcohols in the 19th century. Here, lack of an understanding of this progression has resulted in frequent misattribution of the discovery of alcohol to Muslim philosophers. Other important examples include the changing meanings of the terms *polymer* and *plastic* (21, 22).

In terms of the application of statistics to the history of chemistry (23), a representative example includes the 1985 study by Arnold Thackray and coworkers that attempted to reveal trends in statistical series related to chemistry in America during the period of 1876-1976 (24). In the process, these trends could be used to create what they referred to as "chemical indicators." Such indicators and the complied data could then be applied to a deeper study of the associated history of the field during this time period.

STS as an Emerging Multidisciplinary Field

Beginning in the 1960s, a new multidisciplinary effort emerged that combined various disciplines within the humanities and social sciences (history, anthropology, sociology, political science, philosophy, etc.) in an effort to study how society, politics, and culture affect scientific research, as well as how science and technology affect society, politics, and culture (25-27). These efforts resulted in the production of a new multidisciplinary field typically referred to as science and technology studies or STS (25-28). While STS is often considered a separate discipline from the history of science itself (25, 27, 29), there is considerable overlap between the two fields and STS plays a significant role in the multidisciplinary study of the history of science (29). Of particular interest to historians of chemistry has been the STS topic of technoscience, which focuses on the inseparable connection between science and technology (30).

Multidisciplinary Approaches Incorporating Chemical Analysis and Experimentation

Beyond the more traditional, humanities-based multidisciplinary methods discussed above, new approaches have found growing applications specifically within the history of the chemical arts. Perhaps not surprisingly, these have generally involved a greater application of the chemical sciences to the study of this history, with the older of these combining chemical analysis with archaeology to give the new multi-disciplinary field of archaeological chemistry (Figure 1) (31-34). The application of chemical analysis to archaeology dates as far back as early studies by Martin Klaproth (1743-1817) and Humphry Davy (1778-1829), but its significant development is typically traced to the 1920s and 30s with the introduction of instrumental measurement techniques (35). Since then, it has grown into a scientific subdiscipline in its own right and has provided untold insight into the chemical composition of materials and chemical species from antiquity. As a consequence, this has allowed greater insight into the materials and chemical processes involved in early chemical technologies, as well as the historical pathways involved in their development and evolution (15, 31-33).

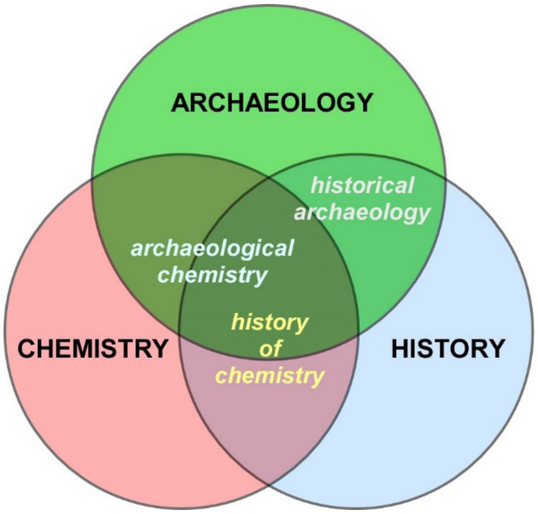

Figure 1. *Overlapping disciplines of chemistry, archaeology, and history.*

Another important new multidisciplinary direction for historical inquiry within the history of science and technology has been the incorporation of laboratory experimentation for the reproduction or reworking of historical processes and experiments (36). As with several of the other multidisciplinary approaches discussed above, such recreations are not a recent development and can be traced to practices such as experimental archaeology, which involved reproducing past constructions, artefacts, and processes. It was in the early 21st century, however, that growing examples of its application to chemistry can be found. Since then, it has grown to be become an important new historical tool to aid in understanding the past and can provide significant new dimensions and insights for historical investigations. Although the application of these methods to the reproduction of alchemical experiments has received the most attention (37-39), particularly with the work of Lawrence Principe (36-38), it has been successfully applied to a number of different processes and time periods (36-42).

New Directions

Scholars of the history of chemistry continue to introduce new methods to its study. Not surprisingly, this includes the application of new disciplines to the study of the history of chemistry. While the goal here is not to be comprehensive, it is worthwhile to highlight specific examples of such additional multidisciplinary efforts.

One new direction that has found some success in applications to archaeology and history has been overlap with the biological sciences, particularly in terms of applications of genomics and genetic testing of archaeological remains. Advances in DNA methodologies have already been applied to archaeological problems, allowing the ability to identify family relations between human remains (43). In terms of more direct application to the history of chemistry, one such particularly interesting example is the efforts of a group of French researchers in 2007 to address various questions concerning timelines in fermentation, impacting the history of leaven bread, beer, and wine (44). Their approach was to study the genetic diversity of the common fermentation yeast *Saccharomyces cerevisiae* via a large-scale evaluation of various yeast populations. In the process, the goal was to determine if there was evidence that strains commonly used for the production of one fermented product could have evolved into strains used for other products, thus establishing a timeline for one fermented product relative to another. Comparison of the genetic relationships of large numbers of bread, beer, and wine strains lead to the conclusion that beer strains were quite poorly related to wine yeast, thus refuting the claim by some historians that grape wine predates the production of barley beer and that beer is an evolutionary product of grape wine (45). Furthermore, such genetic studies led to the proposal that bread strains resulted from a tetraploidization event (chromosome doubling which can lead to rapid mutations) between an ale beer strain and a wine strain, thus leading to the conclusion that bread technology appeared after the production of both beer and wine (44).

Another relatively new multidisciplinary approach has been to incorporate aspects of materials science into the historical studies of chemical species. By using modern material relationships between chemical composition and material properties, it is possible to use the chemical analysis of archaeological artifacts to predict various physical properties of the materials, which in turn can provide insight into how those materials might have been utilized in early societies. Such attempts date back to studies by the glass scientist and historian William E. S. Turner (1881–1963) in the 1920s, but never found significant widespread application (46). More recently, structure-function relationships revealed in Turner's work have been combined with more recent principles of materials science to predict various material properties of glass in an effort to evaluate the validity of narratives in the history of glass, with particular focus on the application of glass to chemical glassware (47). In this study, previously published chemical compositions of colorless Roman, Venetian, and Bohemian glass artifacts were used to predict the material properties of these glasses, including their chemical stability, thermal expansion, thermal conductivity, and density. While the bulk of the predicted properties supported established historical narratives, the analysis of Venetian glass revealed a lack of improvement in thermal expansion compared to previous Roman glass, which suggests that the known improved thermal durability of Venetian glass was due to the removal of physical inclusions as the result of purification of raw materials and not due to any improvements in chemical composition.

Conclusions

As can be seen from the above discussion, the utilization of multidisciplinary research methods is not strictly limited to scientific studies and has been an established practice in both general historical research and especially in terms of the history of science. In addition, just as in the development of scientific research, the extent and diversity of multidisciplinary efforts have increased over time and continue to do so, thus allowing new tools and methods for studies in the history of chemical practice. Furthermore, it is clear that such multidisciplinary efforts provide the same types of benefits to the study of history as previously shown for scientific research. Of course, for such multidisciplinary methods to be effectively applied, this requires either researchers with suitable training in multiple disciplines, or effective collaboration between various practitioners of different disciplines. As such, it is perhaps not surprising that traditional historians with formal chemical training have been especially effective in such multidisciplinary efforts. At the same time, the growing multidisciplinary training included in modern chemistry graduate programs may provide some advantage to those that choose to become chemist-historians, although such chemists could certainly benefit from additional formal training in history. Overall, perhaps the best path forward for the collective study of the history of chemistry is to encourage greater collaborations between chemist-historians, chemical archaeologists, and traditional historians. Such collaborations would thus provide just the collection of discipline-specific training and knowledge that could be most effectively combined for such multidisciplinary historical research.

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COMPUTATIONAL HISTORY OF CHEMISTRY

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Abstract

In this essay it is shown how mathematical and computational approaches can be used to model the underlying mechanisms of historical processes, which transform the structure, dynamics and function of chemistry. By chemical knowledge, I refer to a complex dynamical system emerging from the interaction of the social, material and semiotic systems of chemistry. Besides instantiating some watershed events of the history of chemistry in this framework, the increasing availability of large datasets amenable to computational exploration is discussed, as well as the suitable mathematical theories to carry out these studies. I show how this framework allows for exploring possible alternative histories of chemistry by perturbing its past, leading to solving questions of the sort "what would have happened if." This not only sheds light on the past of chemistry, it rather allows modelling the future of the discipline, with its societal and pedagogical reaches. This approach complements conventional methodologies for the history of chemistry and becomes an interdisciplinary field of research for linguists, mathematicians, physicists, historians and chemists, to name but a few scholars and scientists.

"The search for regularities in human history is becoming a trifle more respectable than it was formerly. That could well portend some significant improvement in our ability to discuss the human future."

—Murray Gell-Mann, 2017 (1)

1 Introduction

The charm of the history of chemistry lies in its convincing, and often literary, narratives of past events whose temporal paths have influenced the evolution of chemistry. History of chemistry shows how the backbone of chemistry emerges from a multidimensional and noisy dynamics of contingencies and certainties. Wonderfully it teaches us about friendships, rivalries, cooperations, academic-industrial alliances, professionalization and technologies, which when embedded in changing social and scientific contexts lead us to the chemistry of the twenty first-century.

History elaborates on the past but it should not be forced to wait until events happen. Its niche lies in the past, but it also includes the present and future, as well as the possible pasts, presents and futures. History spans all tenses. History of chemistry, therefore, ought not beguile us only with the past of chemistry, but with its present and future reaches. Moreover, given the key societal role of chemistry, the history of chemistry endeavors with the past, present and future of our civilization (2).

Tracing back the conditions leading to the discovery of penicillin, or to the development of the Haber-Bosch process is paramount, especially if we want to disentangle the workings of innovation. Similarly, analyzing the conditions facilitating the production and commercialization of thalidomide or the formulation and use of Napalm is extremely relevant to avoid repeating these disasters. These constitute a few examples of the enormous contributions and responsibilities of the history of chemistry. Addressing these questions entails that history of chemistry, at its core, concerns itself with the search for regularities leading to causal relationships (3).

However, most of the historical work, although illuminating, is far from the search for patterns. And this has its own history, as expected. Carl von Clausewitz (1780-1831) and Leo Tolstoy (1828-1910) believed that historical processes were driven by some sort of law, an idea supported by several nineteenth- and twentieth-century historians (4, 5). Nevertheless, the concept of history as a scientific enterprise in the search for patterns lost popularity in the second half of the twentieth-century (6); a movement epitomized by Karl Popper (1902-1994) with his critics to search for historical regularities to foretell the future. Currently, searching for regularities is assumed as a task of the natural sciences, which deal with far less complex systems than those of the humanities. All in all, particles, atoms and genes lack free will, which facilitates the detection of their patterns, while people and their organizations are unpredictable and prone to act upon contingencies. However, scientists are typically busy working within their specialties and very seldom venture beyond their disciplines to seek regularities. Nevertheless, one would expect that chemists, having a strong tradition of detecting patterns, could easily look into their discipline and detect the relevant threads that after being separated from noise would resolve into the driving forces shaping chemistry. The fact of the matter shows that historians are left alone in this central task.

In this essay I argue that Clausewitz and Tolstoy's belief in historical processes driven by patterns is not only a reality but that the moment is ripe to undertake these studies seizing upon present computational and mathematical capacity to delve into the colossal corpus of chemical information gathered to date.

2 History of Chemistry and the Search for Patterns

Historians are very good at devising narratives, often involving causal relationships, where they weave the different dimensions of the historical subject under study. It is gripping to find how nineteenth-century organic chemistry benefited from the strong academe-industry relationship in Germany (7); how professional rivalry hindered the recognition of watershed chemical constructions or theories, for example the frictions between Arrhenius and Mendeleev or between the former and Nernst (8). History contributes to understanding how the deluge of organic chemicals in the first quarter of the nineteenth-century led to devising the molecular structural theory (9), disciplinarily so rooted in our chemical minds. It is fascinating to find that Guyton de Morveau, Lavoisier, Berthollet, de Fourcroy, Hassenfratz and Adet's revolutionary nomenclature (10) was motivated by philosophy of language, which can be traced back to Leibniz (11). These and several other remarkable developments in the history of chemistry evidence how chemistry and its knowledge have been driven by material, social and semiotic aspects of the discipline (2).

Then, in its broadest sense, the history of chemistry entails the temporal analysis of events leading to the status of what has been regarded as chemistry in a given time, this latter discipline understood as the science devoted to transforming matter and theorizing upon it. The events of interest for the history of chemistry involve complex social, semiotic and material factors whose interaction is driven by contingencies and regularities. The question that arises is about the essence of these events. What is the currency of the history of chemistry? I claim it is chemical knowledge.

2.1 Chemical Knowledge, the Currency of History of Chemistry

Jürgen Renn has framed the history of science within a broader history of knowledge (12). This entails considering the history of science as the study of knowledge and of its evolution. In this setting the different dimensions of historical events are integrated into the new object of study: knowledge. Following Renn, Jürgen Jost and I posited that the history of chemistry entails analyzing the evolution of chemical knowledge (2). But, what is knowledge and what is specifically chemical knowledge?

Humans accumulate experiences, which they cognitively structure allowing for predictions of new experiences (13). *Knowledge* entails developing those cognitive structures and predicting, as well as the feedback resulting from predictions (12, 14). When predictions are realized, new experiences are added to the cognitive structures and the predictive method is strengthened. Otherwise, new experiences falling outside the scope of the initial experiences are used to tune the predictive model, while enlarging the cognitive structures. Therefore, knowledge is a dynamical process and it depends on social constraints, such as economic and political interest; as well as cognitive frameworks, which involve theories and meaning generation. Knowledge is stored, shared and transmitted across generations. Thus, it requires a material system to be preserved and spread, for instance through signs and text (2).

Chemical knowledge involves the cognitive structures generated to make sense of the experimentation upon matter transformations. These structures are either used by chemists to estimate future outcomes of their experiments or to modify their cognitive structures in such a manner that they span the new experimental findings. As chemists are embedded in social frameworks, which vary over time and which determine particular ways of thinking (15), their cultures and semiotic systems influence chemical knowledge, which also depends on the materials and technologies available for exploring matter transformations (2).

In our account of the evolution of chemical knowledge we claim that it can be modelled as a *complex dynamical system* made of at least three interacting systems. These are the semiotic, material and social systems (2). As typical systems, they are made of objects and their relationships (16, 17). The objects of the social system include people, academic and scientific societies, committees, enterprises, industries and other forms of social organization, plus computational objects such as robots and artificial intelligence technologies. These social objects are held together by economic, political, cultural, academic and other relations (2). The semiotic system, following Peirce's distinction among objects, signs and interpretants (18, 19), involves substances, reactions and other concepts of chemistry along with their historical representations (signs) that chemists (interpretants) have associated to them (2). These semiotic objects are related by the ternary relation object-sign-interpretant of Peirce's semiotics and by the high-order relations resulting from their combinations (20). The material system is made of substances, reactions, technologies and apparatus, as well as the relationships they establish in the chemical practice (2, 21). Our setting is that chemical knowledge arises from the mutual interaction of the semiotic, social and material systems of chemistry. Chemical knowledge is an emerging property and history of chemistry involves the analysis of the dynamics of this complex object.

So far this does not bring anything new, it sounds just like the use of complex systems jargon to describe what historians of chemistry have been doing for over a century. Nonetheless, this setting brings new possibilities for the history of chemistry. The theory of complex systems regards the emergence of macroscopic phenomena as resulting from multiple relations caused by simple dynamical rules (22), which are often detected through the patterns they form (23). Hence, if by studying past events of chemistry, we detect rules or patterns leading to the rules, we will be in a good position to make predictions and even retrodictions, this latter understood as "predictions" about the past.

The most realistic case of the two mentioned is that of detecting patterns in a large corpus of chemical information about the social, material and semiotic systems of chemistry. If that happens, we have good reasons to think there is an underlying rule driving the historical process. The other case is a bit more difficult, as it involves the direct detection of the rule driving the complexity of the evolution of chemical knowledge. In any case the rule is accepted or rejected insofar as it reproduces the patterns of chemical knowledge.

The first case, that is from patterns to rules, leads to modeling. If we find a pattern in the evolution of chemical knowledge, we may devise a model and let it evolve over time. If the resulting pattern obtained from the model matches that of the historical evolution of chemical knowledge, we have good reasons to take the model as encoding the driving force of the pattern (24). The second case, from model to pattern, is a derivation of the first one. This requires the direct evaluation of the validity of the model by contrasting it with the historical pattern.

Thus, considering chemical knowledge as a complex dynamical system leads to a model, which brings the history of chemistry to new reaches. It allows for estimating the future outcomes of the observed pattern. Interestingly, it also allows for retrodictions by running the model on arbitrary pasts and letting it predict events occurring afterwards but still in the past (2). This is particularly suitable to solve questions of the sort, "what would have happened if." One could ask, for instance, what would have happened with the material and social systems of chemistry, and with chemical knowledge in general, if Berzelius had not devised its notation of empirical formulae. What would have happened if the pre World War I conditions of chemical knowledge had been maintained for longer (25).

In short, the history of chemistry involves the detection of historical patterns in the evolution of chemical knowledge, which we may model as a complex dynamical system arising from the mutual interaction of the semiotic, material and social systems of chemistry. The question that now arises is how to do it. I argue that these patterns are to be detected by analyzing large corpora of historical chemical data through mathematical and computational tools.

3 The Necessity of Mathematical and Computational Methods for Studies in the History of Chemistry

Computational approaches to the history of science have been recently recognized as complementary to the practice of history and sociology of science (26-29). As recently noted by Abraham Gibson, Manfred D. Laubichler and Jane Maienschein (30), history, as a discipline, is currently undergoing a computational revolution. In recent years *Isis* has published some papers on "the computational turn," "the computational revolution" and "the electronic information revolution" (31-33) and in 2019 the journal dedicated a focus section to "Computational history and philosophy of science" (30). In 2017 the annual issue of *Osiris* was devoted to "Historicizing Big Data" (34). In turn, in the *American Historical Review* "the digital revolution" and "the digitized revolution" has been discussed (35). Despite the pros and cons of computation in the practice of history, addressed in the above references, it is clear that "digital sources and computational tools have transformed how we engage with the historical record, including the history of science" (30).

What does this computational turn offer for the history of chemistry and for the search for historical patterns? Computational approaches allow for processing large amounts of historical data and, when coupled with mathematical and statistical methods, for detecting the sought-after historical patterns, if they actually exist. It is important to note that these patterns are not observable by traditional history of science methods, which are often restricted to analyzing periods spanning decades and covering specific geographical regions. Furthermore, such studies typically rely on fewer than hundreds of primary and secondary sources, only some of which are digitized (36). In contrast, datasets for computational studies depend upon millions of digitized records spanning centuries and often the whole globe (37). This change of scale signals a change in the kinds of analysis offered by computational approaches to the history of chemistry.

Furthermore, I propose that mathematical approaches to the history of chemistry promote insights that are otherwise unsupported speculations, or simply unavailable because they are out of reach. For example, the proposal that chemical knowledge is a complex dynamical system involving social, material and semiotic components can be elaborated by employing a suite of mathematical theories for pattern formation, evolution and adaptation, nonlinear dynamics, as well as systems, network, game and collective behavior theories (38). I discuss some particular instances of these theories in section 5. But the central point of mathematical methods for the history of chemistry goes beyond the use of mathematical theories as "canned" tools of straightforward application (2). Rather, I posit that close interactions between chemists, historians, and mathematicians generates fruitful interdisciplinary work while also stimulating some surprising insights into the history of chemistry (39), a topic further discussed in section 6, below. Some of the aforementioned theories are instrumental for detecting patterns and analyzing statistical properties. The products of such combined mathematical methods allow us to glimpse the future of chemical knowledge.

A case study of the mathematical and computational approach to the history of chemistry follows.

4 The Evolution of the Chemical Space

Recent studies of the growth of the chemical space provide a case study of patterns in the history of chemistry (40). By chemical space I mean the substances reported over the history of chemistry, which have been extracted or synthesized by chemists, apothecaries, pharmacists, metallurgists and other chemistry practitioners (2, 41). These substances are endowed with a notion of nearness by chemical reactions and therefore constitute a mathematical space (42). Hence, one talks of substances that are closely related by very few synthetic steps, in contrast to the majority of other substances which are far apart in our current knowledge of possible synthesis plans connecting them. Note that the notion of nearness is arbitrary, as one could select other criteria of nearness. For example, substances can be characterized by their molecular structures and their nearness can be determined by the resemblance of their structures (43).

In any case, the chemical space is an important concept leading to new questions. For example: how does it grow? How rapidly? How are its dynamics affected by social perturbations such as wars or pandemics? Is it perturbed by semiotic changes? Moreover, can we model its evolution? Which are the rules driving its dynamics?

In 1963 de Solla Price briefly discussed the annual report of some chemical starting materials and the growth of chemical elements (44). The first complete account of the growth of the chemical space was reported by Joachim Schummer in 1997, who analyzed the period 1800-1995 by manually screening the indexes of eight printed sources, including handbooks of organic and inorganic chemistry (45). He found an exponential growth with an annual growth rate $r = 5.5\%$, indicating a doubling time of about 13 years. A further study analyzed the growth of organic substances by computationally treating the Beilstein database for the period 1850-2004 and an exponential growth was also found, with $r = 8.3\%$ before 1900 and $r = 4.4\%$ afterwards (46).

In a more recent account, we analyzed 16,356,012 reactions and 14,341,955 substances published between 1800 and 2015 in chemical journals, gathered in the Reaxys electronic database. We found that the chemical space has historically grown at an exponential rate, with a stable growth rate ($r = 4.4\%$) (40). This indicates that about each 16 years chemists have doubled the number of new substances reported. The speed of this rapid chemical production can be expressed in these terms: the number of new chemicals reported by the chemical community in 2015 roughly amounts to all substances reported between 1800 and 1992. That is, in a single year of contemporary chemistry, chemists produced the same number of new substances as reported in 192 years of the history of chemistry. This is the dramatic speed at which the chemical space grows (47)!

In our model of chemical knowledge as a complex dynamical system, we claim that chemical knowledge is driven by the mutual interaction of the semiotic, social and material systems of chemistry. Evidence of these interactions, at least in their binary forms, have been already reported and discussed in (2).

We found that the expansion of the chemical space has been affected by social setbacks such as World Wars (WWs) (40). We observed two drops in chemical production around WWs and quantified the effect of these events in the annual output of new chemicals. It was found that WW I sent back chemical production 37 years, while WW II 16 years. The dramatic effect of WW I follows from the centralized structure of chemistry in the first quarter of the twentieth century, whose capital was Germany. WW I actually motivated a restructuring of chemical industrial and research production, prompting a decentralization in which the USA began to take the lead. By the time of WW II, the social system of chemistry had changed and production was sufficiently less centralized such that, to a large extent, WW II did not affect the annual output of new chemicals.

An interesting semiotic event leading to changes in the material system of chemistry was the introduction of the molecular structural theory (2). This theory solved a semiotic crisis, mainly driven by the deluge of organic substances brought about by the improvement of analytical methods of the early nineteenth-century (48, 49). Before chemists gained control over organic substances, their extractions and synthesis, chemical knowledge was mainly driven by inorganic chemistry (49, 50). Therefore, its semiotics and theoretical structure was tailored to these substances. In this period, for instance, the Berzelian dualistic theory became a paper tool to understand the chemical space and to keep expanding it (48).

At any rate, the 1830s and 1840s brought a growing number of organic substances, which challenged the dualistic formulae of Berzelius and the way of thinking these formulae incorporated in the chemistry of the first half of the nineteenth century (2, 48). Finding a growing number of very different substances with the same composition was totally unexpected, for instance. The introduction of the molecular structure as a new semiotic object of chemistry added a new dimension to the Berzelian algebra of formulae and to the Lavoisian concept of classes of substances (2). Chemists had a new and powerful paper tool at their hands, a topological one where elements hold relationships through chemical bonds. Molecular structures added to the visual character of chemistry and, as Berzelian formulae, became a way of thinking for expanding the chemical space (2).

Our data-driven study of the evolution of the chemical space, besides revealing a stable historical growth, one not halted by social setbacks such as WWs (51), showed other patterns and sharp transitions. This is a further instance of a result attainable only by applying mathematical and computational tools to vast corpora of chemical information. By analyzing the variability of the annual output of new chemicals, we found three clear statistical regimes of chemical production, the first one spanning the period 1800-1860, the second running between 1860 and 1980 and the third and present one beginning in 1980 (40).

Typically, growth studies involve analyzing growth as the slope of the growth curves. However, in our interdisciplinary work, we were fortunate enough to bring mathematicians to our study, for example experts in time series analyses, who indicated to us the importance of the variability of the signal. Duc H. Luu found three statistical regimes where the variability of the annual output of chemicals has been normally distributed (40). These are the three statistical regimes just mentioned, which are characterized by an emphasis on inorganic chemistry before 1860, where the variability of the annual output of new chemicals was the highest in the history of chemistry. This indicates an exploratory regime of the chemical space, where some years brought several new substances and some others not so many. It is clear that the size of the chemical community also played a major role.

By 1860 there was a drastic reduction of the variability, which we argued was caused by the widespread introduction of the structural theory that regularized chemical production, assisted by an ever growing chemical community, which was benefiting from the positive public image of chemistry and of its important chemical industry (9). The interplay between a powerful chemical theory and the social conditions led to regularize the annual output of chemicals, which were mostly organic substances. This trend lasted more than a century—impressively, with two WWs in between! It is noteworthy that WWs did not delay chemical production as observed in other disciplines according to their bibliographic production (44), but rather caused a drop in production followed by a rapid recovery after WWs, leading chemical production to pre-WWs trends (40). This is what Schummer has dubbed as a *catching-up phenomenon* (45). Although he has explored the role of the size of the chemical community in this effect, further work is needed to gauge the dynamics of these postwar recoveries.

A second sudden reduction of the variability of the annual production of chemicals was observed around 1980, but it is still an open question as to the leading event or collection of events causing this further regularization of the variability. It could be caused by the increasing computerization of the chemical practice or a delayed effect of the widespread adoption of spectroscopic chemical instrumentation that took place in the 1950s. At any rate, this third regime of chemistry was characterized by a revival of compounds containing metals, specifically organometallics, followed by a surge of substances of biological interest (40).

Having discussed the mathematical and computational analysis of the evolution of the chemical space, I now turn to discuss the data and methods we have, and we expect to have, to further extend the computational history of chemistry.

5 Data and Methods

Chemistry is the science with the largest output of publications (2) associated to its material practice. Therefore, it is not short of data. Moreover, chemists have developed a strong tradition of data curation, annotation, storage and dissemination initiated by the encyclopedists of the thirteenth century such as Batholomaeus Anglicus (before 1203-1272), Vincent of Beauvais (c. 1190- c. 1264) and Albertus Magnus (1193-1280) (49) and continued by towering nineteenth-century figures such as Leopold Gmelin (1788-1853) and Friedrich Konrad Beilstein (1838-1906). The efforts of these pioneers, plus the colossal amount of new chemical data of the twentieth and twenty-first century are today at our fingertips through electronic databases, which besides being a source of chemical information, constitute an important corpus of historical information.

A well organized electronic database of proven use for history of chemistry is *Reaxys*, owned by Elsevier, and a further one is *SciFinder* hosted by the American Chemical Society. These sources offer important information about the material system of chemical knowledge, which includes substances, reactions, substance properties and reaction conditions. This data is also associated to authors and to their affiliations. Hence, these databases may be used as a source of data for the social system of chemistry as well. As most of the reactions stored in these sources contain details about how the reactions were performed, these databases contribute to the corpus needed to explore the semiotic system of chemistry (2).

Despite the advantages of the chemical databases, historians still lack a well organized and curated database of information about the semiotic and social systems of chemistry. In (2) we mention some reliable sources which could be used to build up such historical databases, which include other electronic databases such as the *ISI Web of Knowledge* and *Dimensions*. However, these databases do not convey a complete picture of the social and semiotic systems. The methods of historians are needed to collect, curate and digitize, for instance, membership in chemical societies, chemical industries and registration records of academic institutions, if the aim is building up a complete database for the semiotic and social systems (2).

Perhaps the most challenging system is the semiotic one, because gathering its data requires developing standards for selecting and curating information. For example, it is important to define what counts as a diagram, table or reaction scheme in historical records. This entails going beyond a formal definition as it has to account for the natural evolution of these terms and concepts. A further question concerns the storage of these data: should they be saved as images? Or is it better to convert them into a machine readable format regardless of whether it is human readable (52)?

Here we must briefly examine the history of codification of molecular structures and reactions. In the 1950s chemists started to ponder the problem of computational encoding of molecular structures (53), which led to connection tables, later on to SMILES and today to InChIs (2, 54). These frameworks were mainly adjusted to encode organic molecules, therefore presenting difficulties for encoding organometallic or inorganic compounds (2). Moreover, they are based on the "chemistry" of the molecules, as encoded in their molecular structures, which disregards several dimensions of their semiotic load. For instance, the intention of the chemist who draws one particular shape, among many possible alternatives to represent a molecule, is lost in these encodings. Fortunately, the growing computational memory and processing capacity is making it possible to store and process molecular structures as images (55), which are coupled with machine learning algorithms to advance chemical knowledge, nevertheless mainly concentrated on the material system. We consider this an opportunity to use current computational power and algorithms to collect chemical information of relevance for the semiotic system of chemistry, and, in general, for the evolution of chemical knowledge.

In (2) we discuss different computational and mathematical methods we find appropriate for studies on the history of chemistry. I have mentioned how time series analysis becomes a powerful tool to analyze historical data. The quality of results obtained through these methods depends to a large extent on the temporal resolution of the data. In section 4 we show the application of these methods to data with annual resolution. Current publishing speeds and editorial policies are making it possible to think about continuous sources of data, which will sharpen the possibilities of time series analysis methods (56). A time series analysis study takes a random temporal signal allowing for studying temporal trends and forecasting (57), as well as detecting changes and evolving behaviors (58). This technique has been recently recognized by historians of science as a suitable method to assist their narratives and to find causal relationships (59).

A powerful collection of mathematical techniques is found in statistical physics that involves the dynamic behavior of mathematical structures, such as graphs and hypergraphs (60-62), which I further discuss in section 6. In general these structures are suitable models for chemical knowledge and its constitutive systems. The general idea is to define a set of objects of study and some relations among them of interest for historical study. Hence, for the material system one may think about analyzing how substances relate to each other through chemical reactions and how that structure of reactions has evolved over time. Likewise, one may consider the dynamics of the social structure of chemistry relating people and institutions as well as the temporal behavior of the connections between concepts and other semiotic tokens of chemical knowledge. Graphs, and in general hypergraphs, are perfectly suited to study the dynamics of the relationships between the systems of chemistry from which chemical knowledge emerges (2).

Another important tool is agent-based modelling, which is used to model simple local interaction patterns and to understand the emerging global complex dynamics. Thus, these models are especially appropriate for understanding the evolution of chemical knowledge. Besides allowing for estimations, agent based models become relevant to study retrodictions, for example, of competing narratives in the history of chemistry (2).

Text analysis tools as well as natural language techniques become important parts of the computational tools for the history of chemistry. These techniques allow for detecting concepts and topics of importance throughout the evolution of chemical knowledge which can be applied, for instance, to treat large corpora of chemical abstracts and reaction details. Therefore, these techniques are applicable to each one of the systems of chemistry (social, semiotic and material) as well as to our exploration of their mutual interplay (2).

A further tool historians can profit from is machine learning, which runs through large databases allowing for predictions, for example through regression techniques, or for classifications. These algorithms also involve reinforcement learning, where the algorithm make decisions based on rewards that it intends to maximize (2).

Bayesian networks constitute a powerful tool for the practice of history of chemistry as they provide a formal setting to explore causal relationships (63), of utter importance for weaving historical narratives. In this setting a time series signal is perturbed and the temporal propagation of the perturbation is analyzed (2).

Some other computational tools and mathematical settings are discussed in (2), but nothing restricts the use of others and the development of new ones motivated by questions from the history of chemistry.

6 Mathematics Triggered by Research on the History of Chemistry

Two questions that computational history of chemistry may address, which I have so far not discussed, are: can we model the evolution of chemical space? What are the rules regulating its dynamics? The answer to the first question is "yes, we can" and we are working on gauging the right model for the evolution of the chemical space. With information about the use of substances to expand the space we can propose statistical models based on the dynamics of chemical reaction networks, described as hypergraphs. In (40) we analyzed whether there are statistical patterns in the way chemists combine their substrates in chemical reactions. We found that although a large part of chemistry is exploratory, that is chemists combine new chemicals with other new chemicals to produce novel substances, there is also a high degree of conservatism in the expansion of the chemical space. We dubbed this trend as the *fix substrate approach* and it entails reactions of very well known substrates, such as acetic anhydride, with new substances (64). Thus, as we know the statistical patterns of the annual participation of substrates in reactions, we can model the expansion of the chemical space. The estimated space can therefore be contrasted with the actual chemical space as recorded, for instance in Reaxys. The mathematical setting to encode participation of substances in chemical reactions is that of hypergraphs, which may be regarded as belonging to the field of network science. What follows is a detailed discussion of how these mathematical structures afford this encoding and how history of chemistry questions have triggered mathematical research in this area.

The success of network theory as a suitable model for systems of an ample range of disciplines has not left chemistry untouched. Collaboration networks and relationships among disciplines are but a few examples of uses of networks to analyze cases of chemical interest. An interesting case at the core of chemistry is Schummer's claim that the logical structure of chemical knowledge corresponds to a network of substances related through chemical reactions (65). This is what today is dubbed as a chemical reaction network. Graph theory has become the mathematical setting of choice for modeling networks (66). In a graph (or network), the objects of the system under study constitute the vertices (or nodes) of the network and the different relationships among objects, the edges of the network. A familiar graph-like chemical concept is that of molecular structure. In this setting, atoms and bonds, respectively, correspond to vertices (V) and edges (E) of the graph, which embodies the molecular structure. A graph G is the couple (V, E). As in a typical molecule, where pairs of atoms are bonded, in a graph, edges connect pairs of vertices (67).

Not surprisingly, graphs have been used to model networks of chemical reactions (46). However, Klamt, Haus and Theis showed in 2009 that these structures miss an important piece of chemical information when used to model chemical reactions (68). As it is well known, reactions typically entail sets of substances. That is, a collection of substrates, solvents, catalysts, which are typically heated and stirred to end up with a mixture of products, which are later on diligently separated and analyzed (69). Klamt, Haus and Theis's argument is that the essential information of a chemical reaction is the AND connector for some substances. We say, A reacts with B to produce C and D, for example, as the result of an experiment (70). Here the important information is that A AND B react together to produce C AND D. If we model this reaction through a substrate-product graph, where substrates are related with products in a directed fashion, that is with arrows from every substrate to each product (71), then we obtain the following relations: A → C, A → D, B → C and B → D. Klamt, Haus and Theis show that this model does not allow for deducing that A AND B are the substrates of the reaction. This occurs because there are further possible interpretations of this model such as that A decomposes into C AND D. The same can be said for the decomposition of B. We can also infer that A AND B react together to produce C through an addition reaction and that under other reaction conditions they produce D. This lack of accuracy of the model, or of several interpretations, multiply as the network grows, that is as more and more reactions are concatenated in the reaction network.

Klamt, Haus and Theis provide the solution to this conundrum by highlighting the possibilities of hypergraphs to gauge the essence of the AND relation of chemical reactions. The basic idea is that reactions simply relate sets of substrates with sets of products. Hence, we talk of {A, B} → {C, D} as a suitable reaction model emphasizing the direction from the left hand side set of substrates to the right-hand side set of products. The main difference between graphs and hypergaphs is that while graphs depict only relations between pairs of elements, hypergraphs do it for sets of elements of any size. As seen, hypergraphs are a novel concept in chemistry and it is also of recent appreciation in mathematics (72), where the attention has been mostly on graphs and their mathematical and statistical properties (73). Nevertheless the further study of these properties for hypergraphs is gaining momentum, in part, motivated by efforts to model large networks of chemical reactions. Interestingly, hypergraphs are a generalization of graphs in such a manner that all that is known about graphs should be reduced to a single case of a general theory of hypergraphs (74). This is an example of mathematics triggered by the study of the history of chemistry. In fact, the study of directed hypergraphs, such as chemical reactions, is just beginning and constitutes a niche of vibrant mathematical research motivated by chemical questions (75).

These mathematical studies may shed light not only on the very concept of chemical space but on the whole of chemical knowledge, as we have argued that the most suitable model for studying the interaction of the three systems of chemical knowledge is a hypergraph. The dynamics of hypergraphs allows for exploring arbitrary moments in the temporal unfolding of chemical knowledge, that is, they lead to predictions and retrodictions, which I discuss in the next section.

7 Predictions and Retrodictions

Detecting statistical patterns in the history of chemistry enables the historical endeavor of the chemical practice to extend beyond the past by allowing extrapolations. It further allows perturbing the past to come up with alternative pasts, presents and futures of chemistry. All in all, statistical patterns in the history of chemistry allow for simulations, predictions and retrodictions.

In 2005 Grzybowski and his team modelled chemical prices based on the use the chemical community made of substances (46). They found that the price of a chemical rapidly decreases with both, the number of synthetic ways of producing it (k_{in}) and the number of uses the substance has as starting material of other chemicals (k_{out}). In fact, the cost follows a power-law distribution that is proportional to k^{-v}, with k being either k_{in} or k_{out} (46). This research was conducted with a fraction of the known chemical space, namely the organic chemical space between 1850 and 2004. Hence, these trends apply to prices of organic chemicals. The same team found that chemists have traditionally used organic substrates of 150 g mol^{-1}, on average, to produce substances with an average of 250 g mol^{-1} (in 2004) (46). This pattern may shed light on the large scale trends of organic chemistry. However, further statistical tests need to be conducted to analyze the reliability of possible estimations.

In section 4 we discussed an important pattern in the evolution of the chemical space, namely that for more than 200 years the growth rate of the chemical space has been stable, with doubling times of about 16 years and with variabilities that have been reducing over time. This trend allows us to predict an expansion of chemical space at a similar pace (76). This leads us to think that an extrapolation is possible and that eventually we could know when, for instance, a specific number of new chemicals would be afforded. However, even if the present variability of the annual output of new substances is the lowest, still the uncertainty of the estimations is high (40). This result shows two important things: i) that extrapolations must be supported by sound statistical analyses to avoid oversimplifications and ii) that estimations of the expansion of the chemical space are complex, presumably calling for information from the social and semiotic systems of chemical knowledge. This latter point highlights the relevance of building up strong social and semiotic databases to foresee the future of the discipline.

A further possibility for computational history of chemistry lies in the retrodictions it permits. This basically entails perturbing past historical data to observe the effects upon subsequent events of that arbitrary past. We conducted a retrodictive study when analyzing the influence of the chemical space upon the evolution of the periodic system (77). In that study we took the known chemical space between 1800 and 1869, with annual resolution, and by taking several systems of atomic weights in vogue in that period, we perturbed the chemical space to obtain the possible periodic systems that several leading chemists such as Dalton and Berzelius may have devised if they had attempted to do so with the chemical space at their disposal (78). We also analyzed how the chemical space by the time of Gmelin, Meyer, Odling, Hinrichs and Mendeleev influenced the systems they reported (79). This allowed us to calculate the false positives and true negatives rates for these chemists by contrasting the periodic systems obtained from the chemical space and those reported by them.

8 Conclusions and Outlook

The increasing amount of data and of computational power are turning computational approaches into an integral part of the historians' tools, which when combined with mathematical insight open new possibilities for the practice of history of chemistry. Here I have shown how computational history of chemistry provides new ways to solve historical questions and allows for asking and solving novel questions related to large scale historical patterns.

Arguing that the currency of the history of chemistry is chemical knowledge, I show how a computational history of chemistry sheds light on the evolution of knowledge by regarding it as a complex dynamical system made of the mutual interaction of the social, semiotic and material systems of chemistry.

Different sorts of data available to undertake studies belonging to the setting here presented are analyzed, as well as several methods and theoretical frameworks assisting those studies. Likewise, I discuss the rich sources of information for the material system of chemistry, vastly documented in chemical databases, and I emphasize the lack of databases for the social and semiotic system. I argue that this is actually an opportunity for the history of chemistry, rather than a limitation, where historians can decide on the sorts of data relevant to curate and to preserve as well as their formats. Clearly, historians cannot create these databases alone; they will require the support of computer scientists and chemists, neither of which alone can come up with databases of relevant use for the history of chemistry.

Computational history of chemistry therefore requires above all interdisciplinary work and constitutes an interesting research niche at least for historians of chemistry, chemists, physicists, computer scientists, mathematicians, philosophers and semioticians. As discussed in (2), the success of these approaches depends, more than on data and methods, on the common and synchronized work of different disciplines, which requires being able to understand the language and jargon of other specialists and even other ways of thinking. All in all, the success of this setting for the history of chemistry is a matter of interdisciplinary respect and of interdisciplinary thinking.

Besides interdisciplinary research, the approaches here discussed also involve interdisciplinary research assessment. That is, when refereeing a publication or research proposal of this sort, a traditional historian, with little knowledge of computation, data analysis or the mathematical techniques discussed, will face problems, as she/he cannot go beyond the validity of the historical question and the kind of data suitable for the study. Likewise, computer scientists, mathematicians and chemists cannot go beyond judging the methods, tools and logic of the subject under study (80). A complete and holistic evaluation of research in this field requires the common work of different experts, with coordinated communication among them during the assessment process.

The success of novel outcomes discussed in this essay necessitate ready access to databases and adequate computing capacity. Traditional history of science departments do not count on computational resources and when these are available, they normally do not offer the minimal conditions of memory and processing capacity to handle large corpora of chemical information. Moreover, they typically do not count on system administrators in charge of machine and software updates. Therefore, alliances between computer science departments and history and chemistry ones are essential.

Based on an analysis by Daniel J. Cohen and Roy Rosenzweig of the pros and cons of computational history (81), in general, the approach here presented solves several issues of the traditional practices of history of chemistry. It brings almost unlimited storage capacity, as information is stored in electronic form. Traditional storage capacities are driven by library and archive capacities of printed records such as books and letters. In contrast, a colossal amount of information can be stored in tiny computer memories. Another advantage is the accessibility to information. This is already evident when consulting century-old printed records by searching, for instance in the Internet Archive. Several users can get direct and simultaneous access to the same records without leaving their desks (82). Computational history of chemistry also offers flexibility, as digital information may be converted into different formats, ranging from text and image to audio and video. One can, for instance, think of recorded interviews of leading chemists or even politicians, which are stored as sound but can easily be transformed into text. Graphical abstracts and videos of current publications also enlarge the possibilities of the data sources for the historical practices of the present and the future.

Disciplinary diversity is a further advantage of the mathematical and computational approaches. The very fact of accessibility to the information makes it possible that not only historians can access the archives, but also practicing chemists and other scholars and scientists with interests in the history of chemistry. Large repositories of information for historical studies contribute to the manipulability and searchability of information we have become accustomed to in the current information era. It is almost unimaginable to search for a particular string of characters in hundreds of handwritten records of the Hellenistic, Chinese or Arabic alchemy without computational aid. Computation has turned this task into a customary process, where segmentation and optical character recognition techniques allow for rapid and efficient queries. The approaches here presented also offer the possibility of interactivity, where databases can be fed from different sources, by different specialists (and even laypeople as in the case of Wikipedia) and the different users can interact and discuss particular subjects, leaving digital records of their interactions, which constitute sources of further historical inquiry.

Despite the advantages of computational history of chemistry, there are challenges and problems to be faced. One of these is data quality. Building up large repositories of information relies on the common work of several annotators and curators. This practice may sound foreign for traditional historians, which often look for primary sources delving into the archives and rely basically on their own interpretations. The approaches here presented often rely on commercial databases which are regularly updated. These updates may modify records of previous entries, for example information dumped today covering the nineteenth century may vary from another dump from the same database and spanning the same period but performed months later. This occurs because annotators and curators may include new sources, for instance journals not considered before, or patents; or because annotation errors are found and corrected. Although this poses a problem for historical studies, as the historical source may vary, it is actually a minor problem as long as the bulk of the database is not affected. The reason is statistical. If updates and corrections do not change the historical trends, they may be considered as background noise of the signal; otherwise, the previous observed trends correspond to data artifacts, which could have been detected running statistical tests over the data. In any case, it is a good policy to perform regular dumps of the data and run statistical tests to determine whether variations are significant or not.

A further issue of these approaches is the inaccessibility to some of the relevant data. Computational history of chemistry requires accessing large databases, some of them owned by private companies or involving costly subscription licenses, which are normally granted to institutions rather than to individuals. Moreover, mathematical and computational approaches require special access to these databases, which go far beyond the limited number of queries allowed to typical users and which often imply dumping the entire database. This issue can be overcome by signing collaboration agreements with database owners. This has been my particular experience with Reaxys, for instance. Providers of other relevant databases such as Clarivate and Digital Science & Research Solutions Inc. offer a variety of similar opportunities for academic partnerships. As mentioned, providing access on individual basis is not the norm, rather, these companies generally grant access to research groups who already have the infrastructure to store and process the information. Typically, a further condition is that access is granted based on a guarantee of information security to avoid data leaks, which may affect the commercial interests of database owners.

A large part of this essay has been devoted to depicting how methods of the natural sciences, especially those devised to look for patterns, find application in the history of chemistry. However, this relationship is far from being unidirectional, and it should be actually taken as a symmetric relation, where historians have a central role in the advancement of the different sciences. As Robin George Collingwood (1889-1943) claimed (83):

> The methods of historical research have, no doubt, been developed in application to the history of human affairs; but is that the limit of their applicability? They have already before now undergone important extensions: for example, at one time historians had worked out their methods of critical interpretation only as applied to written sources containing narrative material, and it was a new thing when they learnt to apply them to the unwritten data provided by archaeology. Might not a similar but even more revolutionary extension sweep into the historian's net the entire world of nature? In other words, are not natural processes really historical processes, and is not the being of nature an historical being?

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20. An example of this ternary relation is the association of the sign "water" to the colorless liquid wetting materials, quenching our thirst, flowing in rivers, boiling at 100 °C, dissolving table salt, plus several other features; an association mediated by the interpretant (2). By high-order relations I mean the further relations between ternary related semiotic objects. For instance, a chemical reaction such as

    $A + B \rightarrow C + D$

    corresponds to a high-order relation entailing the ternary semiotic objects A, B, C and D. The ternary relation in A is given by the sign the interpretant has given to this substance, likewise occurs with B, C and D. As we have shown elsewhere (2), a suitable high-order structure for chemical reactions is a hypergraph, which I discuss in section 6.
21. In Ref. 2, we have highlighted the strong relationship between the semiotic and the material systems, as there are semiotic objects which, through experimental evidence, have been introduced as objects of the material system. This is the case of atoms and molecules, first devised as chemical entities lacking physical reality used to advance chemical knowledge. Later experimental results led to the adoption of Avogadro's hypothesis and the kinetic theory of gases, which prompted the introduction of atoms and molecules as material entities of the chemical practice.

See A. J. Rocke, *Chemical Atomism in the Nineteenth Century*, Ohio State University Press, Columbus, 1984.

22. C. Hooker, "Introduction to Philosophy of Complex Systems: A: Part a: Towards a Framework for Complex Systems," in C. Hooker, Ed., *Philosophy of Complex Systems*, vol. 10 of *Handbook of the Philosophy of Science*, North-Holland, Amsterdam, 2011, pp 3-90, https://doi.org/10.1016/B978-0-444-52076-0.50001-8.

23. An example of simple rules leading to the emergence of a pattern is the *game of life* by John Horton Conway (1937-2020). The setting is as follows (A. Adamatzky, *Game of Life Cellular Automata*, Springer, London, 2010, https://books.google.de/books?id=5iz6C0zzWKcC): imagine a graph paper sheet, where every square can be either black (dead) or white (live). The color of each square is determined by the colors of an initial set of squares that one selects at one's will. Each square is surrounded by eight other squares. The rules read that any live square with two or three live neighboring squares survives. Any dead square with three live neighboring squares becomes a live square. All other live squares die in the next generation. Likewise, all other dead squares stay dead. The first generation of squares is created by simultaneously applying the aforementioned rules to every square. Births and deaths occur simultaneously. Each generation depends on the preceding one and the rules continue to be applied repeatedly to create further generations. The Wikipedia article, "Conway's Game of Life (https://en.wikipedia.org/wiki/Conway%27s_Game_of_Life, (accessed 12 Oct. 2021)) depicts interesting visualizations.

24. In practice, accepting a model requires some further steps, such as validating it. This entails, for example, perturbing (or deleting) part of the input data to observe the stability of the model.

25. This was a period with one of the most rapid annual outputs of new chemicals in the history of chemistry, as shown in E. J. Llanos, *et al.*, "Exploration of the Chemical Space and its Three Historical Regimes," *Proc. Nat. Acad. Sci. USA*, **2019**, *116*, 12660-12665, https://doi.org/10.1073/pnas.1816039116.

26. A. Buyalskaya, M. Gallo and C. F. Camerer, "The Golden Age of Social Science," *Proc. Nat. Acad. Sci. USA*, **2021**, *118*, https://doi.org/10.1073/pnas.2002923118.

27. J. Li, Y. Yin, S. Fortunato, and D. Wang, "Scientific Elite Revisited: Patterns of Productivity, Collaboration, Authorship and Impact," *Journal of The Royal Society Interface*, **2020**, *17*, 20200135, https://doi.org/10.1098/rsif.2020.0135.

28. A. Edelmann, T. Wolff, D. Montagne and C. A. Bail, "Computational Social Science and Sociology," *Annu. Rev. Sociol.*, **2020,** *46*, 61-81, https://doi.org/10.1146/annurev-soc-121919-054621.

29. J. Schummer, "The Impact of Instrumentation on Chemical Species Identity," in P. Morris, Ed., *From Classical to Modern Chemistry: The Instrumental Revolution*, Royal Society of Chemistry, Cambridge, UK, 2002, pp 188-211.

30. A. Gibson, M. D. Laubichler and J. Maienschein, "Introduction," *Isis*, **2019**, *110*, 497-501, https://doi.org/10.1086/705542

31. A.-L. Post and A. Weber, "Notes on the Reviewing of Learned Websites, Digital Resources, and Tools," *Isis*, **2018**, *109*, 796-800, https://doi.org/10.1086/701651.

32. M. D. Laubichler, J. Maienschein and J. Renn, "Computational Perspectives in the History of Science: To the Memory of Peter Damerow, *Isis*, **2013**, *104*, 119-130, https://doi.org/10.1086/669891.

33. S. P. Weldon, "Introduction," *Isis*, **2013,** *104*, 537-539, https://doi.org/10.1086/673272.

34. E. Aronova, C. v. Oertzen, and D. Sepkoski, "Introduction: Historicizing Big Data," *Osiris,* **2017,** *32*, 1-17, https://doi.org/10.1086/693399.

35. L. Putnam, "The Transnational and the Text-Searchable: Digitized Sources and the Shadows They Cast," *American Historical Review*, **2016**, *121*, 377-402, https://doi.org/10.1093/ahr/121.2.377.

36. When I state that traditional historical studies concentrate on specific regions and on periods of decades, I am mainly referring to studies leading to journal publications. There are, nevertheless, important publications, mainly books, where historians present large analyses of longer periods and often of global scope. These studies typically rely on journal publications as well as on other secondary sources.

37. Here sizes are relative to the largest possible historical records. Hence, one can take as a reference for the material system all substances, reactions, instrumentation and technologies used in the history of chemistry. Likewise, the size of the records pertaining to the social system is determined by the number of names and personal data of all alchemists, apothecaries, metallurgists and chemists in the history of chemistry as well as their organizations and institutions. It would also require the inclusion of novel technologies such as robots directly interacting with humans in the practice of chemistry. The size of the semiotic system is given by the collection of all semiotic objects devised and used by practitioners of chemistry over the evolution of chemistry. It is in comparison with this scale that I argue that a traditional historical study relies on small datasets, which are nevertheless a subset of the datasets of computational studies.

38. Particular fields of mathematics in play include partial differential equations, cellular automata, artificial neural networks, evolutionary computation, genetic algorithms, machine learning, time series analysis, agent-based modelling, as well as bifurcation, information, (hyper)graph and complexity theories.

39. There exist examples of mathematics motivated by chemistry. For instance, nineteenth-century settings of

molecular structures as mathematical objects contributed to graph theory with the works of James Joseph Sylvester (1814-1897). Likewise, Arthur Cayley (1821-1895), motivated by the question on the number of isomers for some alkanes, contributed to enumerative mathematics, which were expanded by George Pólya (1887-1985) in the twentieth century. Further information on this subject is found in D. J. Klein, "Mathematical Chemistry! Is It? and if So, What Is It?" *Hyle*, **2013**, *19*, 35-85 (http://www.hyle.org/journal/issues/19-1/klein.pdf, accessed 12 Oct. 2021) and G. Restrepo, "Mathematical Chemistry, a New Discipline," in E. Scerri and G. Fisher, Eds., *Essays in the Philosophy of Chemistry*, Oxford University Press, Oxford and New York, 2016, ch. 15, pp 332-351, doi:10.1093/oso/9780190494599.003.0023.

40. Llanos, *et al*. (Ref. 25).

41. Restrepo, "Das periodische System..." (Ref. 17).

42. Although there is no unique definition of mathematical space, this concept encodes the idea of a set endowed with a notion of nearness. For example, if nearness is associated with distance, then we talk about metric spaces. If it is associated with relationships among elements, then this remits to topological spaces.

43. This is, for example, the basis of the Quantitative Structure-Activity Relationship paradigm.

44. D. J. de Solla Price, *Little Science, Big Science,* Columbia University Press, New York, 1963.

45. J. Schummer, "Scientometric Studies on Chemistry I: The Exponential Growth of Chemical Substances, 1800-1995," *Scientometrics*, **1997**, *39*, 107-123.

46. M. Fialkowski, K. J. M. Bishop, V. A. Chubukov, C. J. Campbell and B. A. Grzybowski, "Architecture and Evolution of Organic Chemistry," *Angew. Chem. Int. Ed.*, **2005**, *44*, 7263-7269, doi:10.1002/anie.200502272.

47. A natural question is how this speed compares to those of other spaces, for instance biological spaces. In this case, one has also to account for rates of extinction and of mutation. See J. W. Bull and M. Maron, "How Humans Drive Speciation as Well as Extinction," *Proc. R. Soc. (London) B*, **2016**, *283*, 20160600, https://doi.org/10.1098/rspb.2016.0600.

48. U. Klein, *Experiments, Models, Paper Tools: Cultures of Organic Chemistry in the Nineteenth Century*, Stanford University Press, Stanford, CA, 2003.

49. H. Leicester, *The Historical Background of Chemistry*, Dover Publications, 1971 (first published Wiley, 1956).

50. W. H. Brock, *The Norton History of Chemistry*, W. W. Norton and Company, New York, 1993.

51. See below in this section for a discussion on the recovery after WWs.

52. Discussing these and other related questions was one of the main reasons we organized the recent *Computational approaches to the history of chemistry* meeting (Max Planck Institute for Mathematics in the Sciences, Leipzig, March 2021), where historians, chemists, computer scientists and mathematicians analyzed different aspects of data driven approaches for the practice of history of chemistry. It was clear that more work is required to advance the construction of electronic databases for the social and semiotic systems of chemistry.

53. L. C. Ray and R. A. Kirsch, "Finding Chemical Records by Digital Computers," *Science*, **1957**, *126*, 814-819, doi:10.1126/science.126.3278.814.

54. Connection tables are lists of atoms and bonds belonging to a molecular structure with further information such as coordinates in a two- or three-dimensional space. SMILES (Simplified Molecular-Input Line-Entry System) are string representations of molecular structures. International Chemical Identifiers (InChIs) are strings used to encode as much as possible information about chemical substances, which include their associated molecular structures.

55. J. Staker, K. Marshall, R. Abel and C. M. McQuaw, "Molecular Structure Extraction from Documents Using Deep Learning," *J. Chem. Inf. Model.*, **2019**, *59*, 1017-1029, https://doi.org/10.1021/acs.jcim.8b00669.

56. Publications before the digital era had regular discrete outputs ranging from annual to weekly, a periodization that is becoming more continuous with the advent of preprint servers and with the online publication of papers right after acceptance, while proofs are edited (2).

57. Z. Wu, N. E. Huang, S. R. Long and C.-K. Peng, "On the Trend, Detrending, and Variability of Nonlinear and Nonstationary Time Series," *Proc. Nat. Acad. Sci. USA*, **2007**, *104*, 14889-14894, https://doi.org/10.1073/pnas.0701020104.

58. D. Brillinger, "Time Series: General," In N. J. Smelser and P. B. Baltes, Eds., *International Encyclopedia of the Social and Behavioral Sciences*, 15724-15731, Pergamon, Oxford, 2001, https://doi.org/10.1016/B0-08-043076-7/00519-2.

59. M. D. Laubichler, J. Maienschein and J. Renn, "Computational History of Knowledge: Challenges and Opportunities," *Isis*, **2019**, *110*, 502-512, https://doi.org/10.1086/705544.

60. A. Aleta and Y. Moreno, "Multilayer Networks in a Nutshell," *Annu. Rev. Condens. Matter Phys.*, **2019**, *10*, 45-62.

61. M. M. Danziger, I. Bonamassa, S. Boccaletti and S. Havlin, "Dynamic Interdependence and Competition in Multilayer Networks," *Nature Physics*, **2019**, *15*, 178-185.

62. P. Chodrow and A. Mellor, "Annotated Hypergraphs: Models and Applications," *Applied Network Science*, **2020**, *5*, 9.

63. J. Pearl, *Causality*, Cambridge University Press, Cambridge, UK, 2009.
64. This finding goes hand in hand with others indicating also preferences for some particular reactions to explore the chemical space, actually the space of substances of potential pharmacological interest. In this case, for example, Suzuki-Miyaura is one of the preferred reactions since 1980 (D. G. Brown and J. Boström, "Analysis of Past and Present Synthetic Methodologies on Medicinal Chemistry: Where Have All the New Reactions Gone?" *J. Med. Chem.*, **2016**, *59*, 4443-4458, https://doi.org/10.1021/acs.jmedchem.5b01409.).
65. J. Schummer, "The Chemical Core of Chemistry I: A Conceptual Approach," *Hyle*, **1998**, *5*, 129-162, http://www.Hyle.org/journal/issues/4/schumm.htm (accessed 12 Oct. 2021).
66. Sociologists were one of the first to recognize the advantages of graph theory. The same community further extended the mathematical possibilities of these structures, which drew the attention of mathematicians. Graph theory is today a vibrant area of research in discrete mathematics. Although I highlight the important role of sociologists for the expansion of graph theory, I do not disregard the early works of mathematicians such as Leibniz and Euler in presenting instances of graphs and their mathematics.
67. Interesting discussions on the development of chemical graph theory are found in Klein (Ref. 39).
68. S. Klamt, U.-U. Haus and F. Theis, "Hypergraphs and Cellular Networks," *PLOS Computational Biology*, **2009**, *5*, 1-6.
69. This is a very broad depiction of a chemical reaction in solution. One could claim that there are also solid state reactions, or even one-pot reactions and others where the separation process is automated, or others where the evolution of the reaction is monitored in real time through the direct insertion of a probe into the reaction vessel (B. Wittkamp, In Situ Monitoring of Chemical Reactions—a Molecular Video, https://www.chemeurope.com/en/whitepapers/126365/in-situ-monitoring-of-chemical-reactions-a-molecular-video.html, (accessed 12 Oct. 2021)). In any case the general idea of reactions as relating sets of chemicals holds and it is an essential part of what a chemical reaction is.
70. The development of the concept of chemical reaction is of central historical and epistemological relevance for understanding the evolution of chemical knowledge. Much work in this direction is needed, where, for instance, semioticians and philosophers of science may contribute to a large extent. At any rate, Lavoisier initiated chemical semiotics by using chemical equations to describe material transformation in terms of substances undergoing changes (11). Further discussions on alternative ways to describe chemical transformations are found in (2)
71. In graph theory these arrows correspond to arcs.
72. Claude Berge (1926-2002) in the 1970s analyzed several of their properties and discussed their delayed recognition in mathematics: C. Berge, *Graphs and Hypergraphs*, North-Holland Mathematical Library, North-Holland, Amsterdam, 1973.
73. W. Leal, G. Restrepo, P. F. Stadler and J. Jost, "Forman-Ricci Curvature for Hypergraphs," *Advances in Complex Systems*, **2021**, *24*, 2150003, https://doi.org/10.1142/S021952592150003X.
74. In this setting a hypergraph H corresponds to the couple (V, E), where V are the objects and E contains the subsets of V that are related. For example, for the reaction $A + B \rightarrow C + D$, its corresponding hypergraph is $H = (V, E)$, with $V = \{A, B, C, D\}$ and $E = \{(\{A, B\}, \{C, D\})\}$.
75. In (2) we discussed some of the mathematical properties already studied for hypergraphs and some others still to be explored.
76. Our results show no sign of saturation in this expansion, as de Solla Price wrongly anticipated for the whole science in the 1960s (44).
77. W. Leal, E. J. Llanos, A. Bernal, P. F. Stadler, J. Jost and G. Restrepo, "Computational Data Analysis Shows that Key Developments Towards the Periodic System Occurred in the 1840s," *ChemRxiv,* **2021**.
78. The underlying hypothesis of this study is that the chemical space directly influenced the ordering and similarities of the chemical elements, therefore the periodic system. See Restrepo "Compounds Bring Back…" (Ref. 17) and G. Restrepo, "Challenges for the Periodic Systems of Elements: Chemical, Historical and Mathematical Perspectives," *Chem. Eur. J.*, **2019**, *25*, 15430-15440, https://doi.org/10.1002/chem.201902802.
79. These are some of the formulators of periodic systems, ranging from Leopold Gmelin (1788-1853) in the 1840s to Julius Lothar Meyer (1830-1895), William Odling (1829-1921), Gustavus Detlef Hinrichs (1836-1923) and Dmitri Ivanovich Mendeleev (1834-1907) in the 1860s. See E. Scerri, *The Periodic Table: Its Story and Its Significance*, Oxford University Press, New York, 2nd ed., 2019, https://books.google.de/books?id=9x2yDwAAQBAJ.
80. Sometimes, even for computer scientists it is difficult to judge the value of a computational approach as reproducibility may become an issue.
81. D. Cohen and R. Rosenzweig, *Digital History: A Guide to Gathering, Preserving, and Presenting the Past on the Web*, University of Pennsylvania Press, Philadelphia, 2006, available online at https://chnm.gmu.edu/digitalhistory/ available online at https://chnm.gmu.edu/digitalhistory/ (accessed 12 Oct. 2021).
82. One is tempted to argue that this practice contributes to lowering global warming emissions, as trips to consult archives and other sources are reduced to a large extent.

However, the environmental costs of computation are far from being disregarded, as shown in E. Strubell, A. Ganesh and A. McCallum, “Energy and Policy Considerations for Deep Learning in NLP,” in *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, 3645-3650, Association for Computational Linguistics, Florence, Italy, 2019, https://www.aclweb.org/anthology/P19-1355 (accessed 12 Oct. 2021). The question that arises concerns the net environmental costs of the approaches here presented and how they actually compare with the traditional approaches to the history of chemistry.

83. R. G. Collingwood and W. J. van der Dussen, *The Idea of History*, ACLS Humanities E-Book, Oxford University Press, Oxford, UK, 1994, https://hdl.handle.net/2027/heb.05489.

About the Author

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Born in the Same Year as HIST (1922)

- Har Gobind Khorana: January 9, 1922, in Raipur, in the Punjab in (then British) India.
- Robert William Holley: January 28, 1922, in Urbana, Illinois, USA.
- George C. Pimentel: May 2, 1922, in Rolinda, California, USA.
- John Goodenough: July 25, 1922 in Jena, Germany.

Khorana and Holley, born in the same month in widely separated places, shared the 1968 Nobel Prize in Physiology or Medicine for their roles in deciphering the genetic code, the link between nucleic acid and protein sequences. Khorana and his co-workers at the University of Wisconsin-Madison synthesized short chains of RNA which were used to direct the synthesis of short protein fragments. Later Khorana and co-workers made what is considered the first artificial gene. Holley and his co-workers at Cornell University and the US Plant, Soil and Nutrition Laboratory on the Cornell campus, isolated and sequenced alanine transfer RNA, which directs incorporation of alanine into proteins.

Pimentel’s research is well known to physical chemists and his service to chemical education and the chemical profession is widely recognized in the American Chemical Society. Matrix isolation methods and chemical lasers are his main legacies in physical chemistry. He received the highest award of the American Chemical Society, the Priestley medal, in 1989, the year of his death. He had served as ACS president in 1986. The ACS award in chemical education was renamed the George C. Pimentel Award in Chemical Education in his honor.

Goodenough shared the 2019 Nobel Prize in Chemistry for the development of lithium ion batteries, ubiquitous power-storage devices for mobile electronics. Goodenough and co-workers made their key contributions to this technology at the University of Oxford in the 1970s and 1980s. The Materials Chemistry division of the Royal Society of Chemistry have an award named for Goodenough.

HISTORY OF CHEMISTRY AS A TOOL FOR THE ENGAGEMENT OF UNDERREPRESENTED STUDENTS IN CHEMISTRY

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Abstract

How can the history of chemistry be an effective tool for the recruitment and retention of underrepresented students in chemistry? How can the history of chemistry address equity in the classroom? We will explore how the stories of historically underrepresented chemists can be used to attract more diverse students into the discipline.

"I am making [an] application for a Fellowship with the National Research Council for the year 1933-34. I should greatly appreciate if you would kindly write a letter of recommendation for me," Dr. Percy L. Julian wrote to then Harvard Professor Elmer P. Kohler in February 1933 (1). Around this time, Julian's first paper (2) with fellow chemist and colleague, Josef Pikl had just been accepted for publication in the *Journal of the American Chemical Society (JACS)*, a highly prestigious scientific journal. Julian wanted to continue his research efforts at DePauw University and he needed to provide financial support for his aging parents.

> I am compelled to contribute 50 dollars per month to the maintenance of my parents now, and since there are facilities here for work, the library being very complete and since working conditions are so pleasant, I could very well carry out my work, live at home and avoid any suffering on the part of my parents

wrote Julian.

Julian's career as a chemist was quite different from Saint Elmo Brady's, who was the first African American to earn a Ph.D. in chemistry in 1916 from the University of Illinois at Urbana Champaign. Brady spent his entire career teaching at HBCUs (Historically Black Colleges and Universities) mentoring several future chemists during his academic career. A recent publication authored by a former student of Brady's discusses his impact on HBCUs and chemical education (3). After earning his Ph.D. in 1931 from the University of Vienna, Julian was only the third African American to earn a doctoral degree in chemistry and he was determined to engage in cutting-edge research, but obstacles and significant barriers were always in his path.

Kohler responded to Julian a week later (1) emphasizing that he would likely not receive such a fellowship. "If I were you, I should not put too much hope in the outcome," Kohler wrote. Furthermore, Kohler indicated that the fellowships are often provided to give "exceptional young men an opportunity to perfect themselves in their craft." Julian was only 33 years old at this time.

Although Kohler did not say no to Julian's request for a letter of support, he did suggest that the selection process for the fellowship was based on the "qualifications" of a candidate and not race.

> I am writing this, lest should the outcome be unfavorable, you would feel that the Board was acting on prejudice of some kind—prejudice on account of your race, your relations to Howard University, or your preferences for DePauw. None of these matters will be taken into consideration. The application will

> be considered only from the point of view of your qualifications.

Kohler's response actually provides evidence of bias faced by African Americans in the field of chemistry which remains a significant challenge in our society. Kohler's suggestion that Julian's application would be evaluated based solely on merit and not race is completely unreasonable considering that Julian left the U.S. to pursue his doctorate in chemistry because of institutional racism. In fact, Kohler suggested to Julian that there was no place for him in chemistry (4). Dr. Julian continued successful research at DePauw until 1935, when the Board of Trustees refused to grant him a teaching appointment (5). Dr. Julian had an incredible career and made significant intellectual contributions to society publishing over 100 papers in high-impact journals and registering over 100 patents. Imagine what additional contributions Julian could have made to society if he did not experience bias and racism throughout his career?

Figure 1*. Illustration of Percy Lavon Julian by Giulia Lampis.*

Julian had overcome many things in his life at the time he applied for the NRC grant. Born in 1899 in Montgomery, Alabama, Julian attended Alabama schools for African Americans that ended with the 8th grade because of racism, but earned a B.A. (valedictorian and Phi Beta Kappa) from DePauw University in 1920. In 1923, Julian earned an A.M. degree in chemistry from Harvard University, but was denied the opportunity to pursue a doctoral degree at the institution because no Ph.D.-granting university would let him serve as a T. A. (teaching assistant) for White students. Almost a decade later, Julian finally earned his Ph.D. in chemistry.

How can Julian's story of grit and perseverance be used to inspire the next generation of chemists? His story is a powerful example of how the history of chemistry can be used as an effective tool for engagement of BIPOC (Black, Indigenous and People of Color) communities. Julian's remarkable life and career was brilliantly profiled in the 2007 "Nova" documentary, *Forgotten Genius*, which was rebroadcast on PBS in February 2021 during Black History Month (6). Chemistry faculty could use shorter segments of *Forgotten Genius* in the classroom and align the documentary with an organic chemistry curriculum for student engagement (7). Thus, Julian's remarkable accomplishments and achievements can be used as a "history of chemistry engagement tool" to educate all students with an emphasis on BIPOC communities.

Most recently, a Lawrence Technological University (LTU) student documentary entitled, *Women Untold* was shared on YouTube (8) to celebrate the remarkable achievements of three African American women in STEM (Science, Technology, Engineering and Mathematics) including Dr. Jewel P. Cobb, a biologist and president of an R1 university; Dr. Evelyn Boyd Granville, a mathematician who completed orbital calculations for three NASA (National Aeronautics and Space Administration) missions; and Alice Augusta Ball, a chemist who developed the first viable treatment for leprosy (Hansen's disease) in the early 20th century while a faculty member at the College of Hawaii (now known as the University of Hawaii). The film was written, produced and directed by Marie Anne Torres-Lopez, a recent graduate of LTU (9). *Women Untold* is being used as an educational tool to address equity in STEM.

Born in 1892 in Seattle, Washington, Ball earned two undergraduate degrees from the University of Washington: a degree in pharmaceutical chemistry in 1912 and a degree in pharmacy in 1914. Remarkably, in 1914, Ball also co-authored a research paper in *JACS*. These are tremendous accomplishments from Ball before she earned her master's degree from the College of Hawaii and successfully synthesized and characterized the ethyl esters from Chaulmoogra oil for the treatment of leprosy.

Paul Wermager, Science and Technology Librarian at the University of Hawaii, was interviewed in *Women Untold* and discussed the impact of Ball's remarkable scientific achievements. Wermager shared that Ball's accomplishments really emphasize a "certain level of genius" because the research was completed rather quickly. "She did it in such a brief period of time. We are talking months, not years," says Wermager.

Recently, a Lawrence Tech chemistry professor has utilized the documentary *Women Untold* to engage students enrolled in an organic chemistry course. The students were asked to provide their reflections about *Women Untold* on the final exam for the course. An African American student wrote, "This film made me feel great because it gave people that look like me representation. We are often lost and left out of history so it is great to see the conscious effort of our inclusion."

An LTU adjunct professor in the Department of Humanities, Social Sciences and Communication also used the documentary in a seminar course focused on science, gender and race. An LTU African American student enrolled in that course stated,

> This documentary emphasizes the importance of community, education, and exposure. It shows how people of color, more specifically how women of color have made major contributions to STEM despite the unfair treatment they received. It is vital for young Black girls to know that they are supported and that they, too, are capable of achieving excellence within the STEM community.

Thus, this is anecdotal evidence that students find these types of stories to be compelling.

Narrative films such as *Forgotten Genius* and *Women Untold* are merely two examples educators can use to engage students in the classroom. Additional resources teachers can use as educational tools with their students include the American Chemical Society (ACS) Directory of the National Historic Chemical Landmarks (10) and the National Science Foundation supported ScienceMakers section of The History Makers (11). For example, the National Historic Chemical Landmarks website includes brochures on the careers of Brady, Julian and Norbert Rillieux, a chemical engineer who "revolutionized sugar processing with the invention of the multiple effect evaporator under vacuum (12)." The History Makers includes oral histories on several chemists including Jeannette Brown, who was the first African American woman to earn a M.S. degree in chemistry from the University of Minnesota in 1958. Brown, who worked for both CIBA Pharmaceutical Company and Merck also authored the book, *African American Women Chemists* (13), which also can be used as a resource. Educators could allow their students to conduct research using these engaging resources for a history of chemistry storytelling project. Students could work in teams to prepare a creative infographic or narrative video to celebrate the intellectual achievements of chemists from BIPOC communities.

Chemical & Engineering News (C&EN) recently celebrated African American chemists and chemical engineers in a special issue for Black History Month (14). Professor Paula Hammond, Chair of the Department of Chemical Engineering at the Massachusetts Institute of Technology (MIT) served as guest editor of the *C&EN* issue and wrote,

> We have always been present in the sciences—but now more than ever, we must appreciate and acknowledge the presence of Black people and other people of color. We must find ways to continue to raise our voices and celebrate our work. As a nation, we all benefit from the huge talent gained when all are included in the science enterprise.

A significant and novel aspect of this *C&EN* special issue is that current African American chemistry graduate students were given a rare opportunity to interview very accomplished and brilliant chemists, thus providing these young chemists a significant platform to expand their network, which is important for a successful career pathway in the chemical sciences.

Professor Hammond, who is a pioneer in drug discovery applications is emphasizing the importance of representation in the chemical sciences. *Forgotten Genius*, *Women Untold*, the ACS Directory of the National Historic Chemical Landmarks, The History Makers and the special *C&EN* issue celebrating African American chemists are powerful history of chemistry tools that educators and chemistry professors can use to address equity in the chemistry classroom. Including more narratives about African American chemists in the chemistry curriculum is one strategy to help encourage all students to pursue careers in chemistry. Furthermore, this approach can help address barriers to success in STEM including sense of belonging, STEM identity and stereotype threat for students from BIPOC communities. Thus, the history of chemistry *can* and *should* be used as a tool to engage the next generation of chemists.

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References and Notes

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OUT OF OBSCURITY: CONTEXTUALIZING FORGOTTEN WOMEN CHEMISTS

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Abstract

Over the last decade, the past contributions of more and more pioneering women chemists have come to light (1, 2). In this contribution, we will address some of the ways that accounts of the lives of women chemists do, and should, collectively differ from biographical accounts of male chemists.

Conventional biographies of male chemists of the dominant culture, such as in the *Biographical Memoirs of Fellows of the Royal Society of London*, focus almost totally upon their chemical accomplishments (one of the few exceptions being that of Dennis Evans, inventor of the Evans balance (3)). Often, that is because their life-paths were so straightforward: born, educated, academic position, research contributions, died. Detailed context is redundant; the role of others in their life-paths is often minimal or ignored.

To appreciate the accomplishments of pioneering women chemists, it is necessary to see them through the lens of gender. That is, in addition to their chemistry achievements, it is important to chronicle the challenges which they faced in their own time and place. Only by researching and acknowledging these obstacles can we truly appreciate their contributions to the progress of chemistry. In this essay, we will use case studies to highlight some of the generic challenges uniquely faced by early women scientists. For more detailed biographical accounts of these women chemists, the Reader should consult the appropriate reference source.

Background

How did our interest in uncovering the lives and work of forgotten women chemists begin? It all started with a cameo portrait in a book—a portrait of a young woman in among the endless photos of mostly elderly males. The portrait was of Canadian researcher in the field of radioactivity, Harriet Brooks (1876-1933), and the book was *Discovery of the Elements*, by Weeks and Leicester (4). According to the figure caption, Brooks (Figure 1) worked with Ernest Rutherford. Curious, we decided to spend a few weeks researching who she was, and why she was featured in the book. We uncovered some information about her, which led us to archives, which led us to her surviving family, which led us … to a total of two years of research. Finally, we assembled all we could find. With a Canada Council grant towards publication, we submitted the manuscript. It was rejected.

As scientists, we had written "just the facts," focusing largely on university grades, details of her experiments, together with transcriptions of complete letters to-and-from friends and members of her family. It was a historian of science, Marianne Ainley (5), who mentored and taught us how to attempt to think like a science historian. We needed to answer questions such as: Why did Brooks go to university? What was life like for an intelligent young woman in Victorian Canada? Why was there a separate women's college at McGill University at the time? Why would Rutherford take on a young woman as a research student? Why did Brooks go to the Adirondacks? Why did she give up an apparently promising career? Why did she die at a comparatively young age? And many others. After undertaking years of contextual research, we completed our first published voyage into the history of women in science (6).

***Figure 1**. Harriet Brooks (permission, McCord Museum, Montreal, Canada)*

Lack of Educational Opportunities

For male chemists of the dominant culture, gaining an education was never (or rarely) a problem. For women who had become fascinated by some aspect of chemistry, a formal education was sometimes an insurmountable hurdle. Probably the best exemplar is that of the German amateur chemist, Agnes Pockels (1862-1935) (Figure 2). Pockels' research on surface films laid the foundation for subsequent research in the field (7). As a girl, she was fortunate for her time in obtaining an academic grade-school education, where she developed her interest in science. At that time, women were barred from attending German universities, and later, when women were admitted, Pockels' parents forbade her from applying. This did not stop her, as she stated in her own recollections (8):

> I attempted to continue my education by my own devices, first of all by the use of a small text book by Pouillet-Müller and since 1883 by means of books provided by my brother, Friedrich Pockels, who is three years younger than I … who at that time was a student at Göttingen.

Unable to access a laboratory, Pockels used the family kitchen sink. As her sister-in-law explained (8): "In this way, Agnes made her first observations in the field of capillarity." In many of the accounts of women chemists, a male mentor was necessary to open doors barred to a woman who had no academic credentials. In Pockels case, it was Lord Rayleigh. She wrote to him informing him of her research (9):

> Having heard of the fruitful researches carried on by you last year on the hitherto little understood properties of water surfaces, I thought it might interest you to know of my own observations on the subject. For various reasons I am not in a position to publish them in scientific journals …

Rayleigh could well have ignored this communication from an unknown German woman amateur scientist. Instead, he submitted it to the prestigious journal *Nature*, with an accompanying recommendation that it be published (10). The initial communication, co-authored by Rayleigh (11), and a subsequent paper with Pockels as sole author, were duly published (12).

***Figure 2**. Agnes Pockels (Wikimedia Commons, https://commons.wikimedia.org/wiki/File:Agnes_Pockels_ca1892.jpg)*

Lack of Academic Positions

In 1947, the Chemical Society, London, published a book titled *British Chemists* (13). This book contained brief biographical accounts of famous British chemists up to that date: they were all male. Why were there no "outstanding" professional women chemists in the book? The simple answer was that women were rarely permitted to hold academic rank and therefore they occupied the fringes of academia.

As we have described in *Pioneering British Women Chemists: Their Lives and Contributions*, in her early career, Dorothy Crowfoot Hodgkin (1910-1994), Nobel-Laureate-to-be, provided an example of a marginalized woman chemist (14):

> Though Crowfoot had made important contributions to [X-ray crystallographic] science, at the end of the [Second World] War, her rank at Oxford was still only that of a Tutor. Deeply in debt, she realized that most of her male colleagues had university positions,

> as well as research appointments, so she asked Cyril Hinshelwood, Professor of Chemistry, to help her acquire a better position. With his help, Crowfoot was appointed as a University Demonstrator in Chemical Crystallography in 1946, her first appointment as an Oxford University employee.

Lack of Academic Recognition

Chemists, like all scientists, become famous usually by peer recognition, especially by means of awards from professional societies. However, for many national chemical societies, women were barred from even being members or fellows (15). As an example, it took 40 years from the first (unsuccessful) motion in 1880 by Augustus Vernon Harcourt for the admission of women chemists as Fellows of the Chemical Society (London) until the goal was accomplished (16). Even then, it came about through the British Government's 1919 Sex Disqualification (Removal) Act, legislation which removed barriers against women in general (17).

The pathway to recognition of academic exceptionality in Britain came through election as Fellow of the Royal Society. However, the Royal Society was an even greater barrier to the progress of women chemists. Though the 1919 Act removed the barrier in principle, it was not until twenty-five years later that anything transpired. As Hilary Rose wrote (18):

> This extraordinary gap suggests at best a collective amnesia—or perhaps a repression of memory—within the Royal Society, in which the fact of legal eligibility and the political likelihood of success become conflated to become an unstated and legally false, but socially powerful consensus that women were not admissible.

It was an article in 1943, in the British communist-leaning newspaper, the *Daily Worker*, which raised the issue. Evolutionary biologist J. B. S. Haldane was asked for his view on who would be the strongest candidate from the biological sciences. His reply was that biochemist, Marjory Stephenson (1885-1948), was his choice (19): "I think the strongest claim is that of Dr. Marjory Stephenson who was the first person in the world to do work on bacterial metabolism as exact as that on mammalian metabolism …" Stephenson was duly elected as one of the two first women Fellows in 1945 (the other being Kathleen Lonsdale). Had she been elected earlier in her career, Stephenson would likely have been nominated for a Nobel Prize. As it was, her untimely death in 1948, age 63, precluded such an honor.

The Imposter Syndrome

For the "great men," many of them realized that fame would come and they saved their correspondence in the expectation that their letters would be posthumously presented to a university archive. By contrast, for most of the women chemists, there was the assumption that their humble contributions would not be worthy of remembrance, and, for the most part, their letters have long since vanished. A letter of Harriet Brooks to Ernest Rutherford (in whose voluminous correspondence this letter was found) makes the point very succinctly (20):

> I am afraid I am a terrible bungler in research work, this is so interesting and I am getting along so slowly and so blunderingly with it. I think I shall have to give it up after this year, there are so many people who can do it so much better and in so much less time than I that I do not think my small efforts will ever be missed.

Yet Rutherford, himself, had contrary views. He wrote to Arthur Schuster, Head of Physics at the Victoria University of Manchester that (21):

> … next to Mme Curie she [Brooks] is the most prominent woman physicist in the department of radioactivity. Miss Brooks is an original and careful worker with good experimental powers …

The Matilda Effect

A common problem for junior women researchers is that they are subsequently "written out" of the discovery. This can also be true for male co-researchers. In this context it is called the Matthew Effect. The originator, Robert Merton described it as (22):

> … the accruing of large increments of peer recognition to scientists of great repute for particular contributions in contrast to the minimizing or withholding of such recognition for scientists who have not yet made their mark.

The Matthew Effect was named by Merton after the saying in the Bible, New Testament, The Gospel according to Matthew: "For unto everyone that hath shall be given, and he shall have abundance; but from him that hath not shall be taken away even that which he hath."

Convinced that such an Effect was of far greater significance in the case of women scientists, American historian of science, Margaret Rossiter, proposed the use of the term the Matilda Effect to describe the achievements of those women scientists whose work is attributed to their male colleagues (23). This Effect had been first described by suffragist and abolitionist Matilda Joslyn Gage (1826-1898). The Matilda Effect can be illustrated by the work of Brooks when she was working with Rutherford at McGill University, Montreal, Canada. Their research culminating in the discovery of a "new gas from radium" (now known as radon) was published under both their names (24). However, subsequently, at least one account of the discovery was attributed to Rutherford alone (25).

Appropriation

While the Matilda Effect can account for the disappearance of many women chemists from the record, it is dangerous to simply attribute all "disappearances" to one single cause. In other cases, it is because their work has been appropriated. Sometimes the appropriation may have been accidental, but other cases, deliberate. One case of appropriation, which is debatable whether it was accidental or deliberate, is that of the priority of demonstrating the "greenhouse effect" (26). American amateur scientist, Eunice Foote (1819-1888), was clearly the first to do so, though John Tyndall is given credit. As Roland Jackson has commented (27):

> In 1856, an American woman, Eunice Foote, discovered the absorption of thermal radiation by carbon dioxide and water vapour. That was three years before John Tyndall, who is generally credited with this important discovery—a cornerstone of our current understanding of the greenhouse effect, climate change, weather and meteorology. Tyndall did not reference Foote's work.

The most egregious case of appropriation was probably that of Alice Augusta Ball (1892-1916) (28). This young African-American woman chemist had been appointed Instructor in Chemistry at Hawaii College. She was also undertaking research in natural products chemistry towards an M.S. Having such skill in the field, Ball was approached by Assistant Surgeon, Dr. Harry T. Hollman. At the time, the best palliative treatment for Hansen's disease (leprosy) was oil extracted from the chaulmoogra tree. As it was water-insoluble, it could not be given by the preferred means, that of injection.

Hollman asked Ball to convert the oil to a water-soluble form. This she did by converting the parent compounds, fatty acids, to ethyl esters. Many patients' lives were vastly improved by this injectable method. Sadly, Ball died at the age of 24. An account of her death stated (29):

> Just over 100 years ago, as World War I raged in Europe, a chemistry professor named Alice Ball was demonstrating the use of a gas mask when something went tragically wrong. The brilliant, young chemist died a few months later at age 24, likely from accidentally inhaling chlorine gas.

As one of her biographers, Jeannette Brown, recounted (30):

> After her death, Dr. Arthur L. Dean who was a chemist and President of the College of Hawaii continued Ball's research. Large quantities of this new drug were made and distributed to patients worldwide. Dean published his results without mentioning the work of Ball and it became known as the Dean method. Later, in a medical journal publication in 1922, Hollman mentioned the contribution of Alice Ball. Still, it took years before Alice Ball was recognized for her accomplishments. The neglect may have been due to both sexism and racism …

Figure 3. *Alicia Ball (Wikimedia Commons, https://commons.wikimedia.org/wiki/File:Alicia_Augusta_Ball.jpg)*

The Marriage Problem

The termination of a woman chemist's career upon marriage was referred to in earlier times as "matrimonial mortality." Though there are some notable examples of couples collaborating and thriving together (31, 32), even then, the woman usually held a more junior academic position, or none at all. Two examples of the woman chemist holding a more junior rank were both Nobel Laureates: Marie Sklodowska Curie in radiochemistry, and Gerty Radnitz Cori in biochemistry.

From our own research, for the large majority of women chemists, marriage spelled the end of their professional aspirations. As Flora Garry (1900-2000), a graduate of King's College, University of Aberdeen, Scotland, wrote (33):

> 'Learnin's the thing,' they wid say,
> 'To gie ye a hyste up in life.'
> I wis eence a student at King's.
> Noo I'm jist a professor's wife.

The large majority of male chemists married. This enabled the male researchers to "off-load" domesticity and concentrate upon their research. The point was made succinctly by Terri Apter in *Professional Progress: Why Women Still Don't Have Wives* (34):

> A retired woman Lecturer at the University of Cambridge, when asked whether she regretted not marrying, responded that she would have been glad to marry had she only found someone who would have made a good wife.

Some women chemists were able to assist in their husband's career, though their roles have often been forgotten. An early example was Grace Coleridge Toynbee (1858-1946). Following marriage to British chemist Percy Frankland, she continued active research. One of Frankland's obituarists noted (35):

> Probably in few cases have husband and wife collaborated so effectively and enthusiastically in both research and professional work. On one occasion it was said, "Many women in the past have helped their husbands, but Percy Frankland is the first man who had the chivalry to admit it."

The 1920s saw the Lapworth-Robinson "golden age" of organic chemistry at the Victoria University of Manchester. Yet it is rarely mentioned that these two relied heavily upon their spouses, Kathleen Holland (Mrs. Lapworth, 1879-1960) and Gertrude Walsh (Mrs. Robinson, 1886-1954). In a review of the Chemistry Department, it was stated (36):

> An unusual feature of the life of the School of Chemistry at this time was the presence in it of the wives of both professors. Mrs. Lapworth as her husband's secretary helped him greatly with the detail of the heavy administrative responsibilities in the department. Mrs. (later Lady) Robinson, as an Honorary Research Fellow, worked on long-chain acids in the professor's laboratory. Both took a kindly and active interest in staff and students.

For some married women chemists, an active chemistry career required a role reversal. Thomas Lonsdale and crystallographer Kathleen Yardley Lonsdale (1903-1971) provided one such example. Thomas Lonsdale reflected (37):

> When the apple fell on Newton's head someone gathered it and the other windfalls and made a pie for his dinner, thats [sic] my job now a bit, it always has been. … Even before we were married I knew she had one of the most powerful intellects of the time. … I only know enough about her work to realize its importance and value and how fortunate I have been associated with it, "in getting Newton's dinner."

One unique challenge in tracking the life and work of women chemists is that of changing family name upon marriage. As a result, a literature search for contributions would cease at that point in time, not always to be connected to the subsequent married name. Sharon McGrayne has provided one such example, that of Dorothy Crowfoot Hodgkin (38):

> Dorothy published her penicillin studies under her maiden name "Crowfoot" and announced vitamin B_{12} as "Hodgkin." Years later some scientists still did not know that the Crowfoot of penicillin fame was the Hodgkin of B_{12} fame.

For lesser-known women chemists, the link between birth and married names is even less likely to be identified.

The Woman "Super-Chemist" Phenomenon

In cases where women chemists were being considered for an academic position, the bar was often set unreasonably high, excluding them from consideration. Any candidate was expected to be of a caliber far higher than that of a male candidate. Margaret Rossiter described the effect of Marie Curie's visit to the United States in 1921 as raising the bar for American women chemists to unattainable levels (39):

> Before long most professors and department chairmen were … expecting that every female aspirant for a faculty position must be a budding Marie Curie. They routinely compared American women scientists of all ages to Curie, and finding them wanting, justified not hiring them on the unreasonable grounds that they were not as good as she, twice a Nobel Laureate!

In Britain, it was the outstanding woman biochemist, Ida Smedley Maclean (40), who was the benchmark for female hiring. For the position of Reader (Professor) in Chemistry at King's College of Household and Social Science, London in the 1930s, it was stated that (41): "… it would be of great value to the Department to secure the services of a woman with the high scientific standing and personality of Dr. Ida Maclean." It seems highly unlikely that any male candidate for the position would be expected to undergo a "personality" test—or have any benchmark to be compared against.

Importance of Male Supporters

In accounts of HerStory, it is sometimes overlooked that with the constraints of society, women could not make progress without empathetic male mentors or facilitators. In the societal context, this has been discussed in *Traitors to the Masculine Cause* (42). In the context of British chemistry, we have identified Augustus Vernon Harcourt, William Tilden, and others as promoters of the rights of women chemists (43).

Some, such as the biochemist F. Gowland Hopkins, promoted the careers of many British women biochemists (44) (including that of Marjory Stephenson—see above). As Mary Creese has eloquently stated (45):

> At the time when there were practically no women research workers in any of the other university departments at Cambridge, Hopkins gave them places in his, despite the criticism which this brought him. Even in the 1920s and 1930s, when, as a Nobel laureate with a world-wide reputation he received hundreds of applications for places in his laboratory, nearly half of the posts in his Department went to women scientists.

However, as we have established for many female-friendly departments, simply hiring women chemists was not enough. The environment was of paramount importance. J. D. Bernal's crystallography group epitomized such a positive workplace. Dorothy Hodgkin was a member of Bernal's group at the University of Cambridge from 1932 to 1934. In the Obituary for Bernal, written by Hodgkin, she described the very pleasant working atmosphere and convivial lunches (46):

> Every day, one of the group would go and buy fresh bread from Fitzbillies [which still exists in Cambridge], fruit and cheese from the market, while another made coffee on the gas ring in the corner of the bench. One day there was talk about anaerobic bacteria on the bottom of a lake in Russia and the origin of life, another, about Romanesque architecture in French villages, or Leonardo da Vinci's engines of war or about poetry or printing. We never knew to what enchanted land we would be taken next.

It is noticeable that, in our research, comments upon such conviviality in this, and in other research groups (such as Hopkins's), came always from women researchers. It was for them that the working environment particularly mattered.

Where Does One Begin "Discovering" Forgotten Women Chemists?

Whereas with male chemists of the past, there are many, many, compilations of names and research fields, this is not true for female chemists. In our own work, there has not been one definitive route for "discovering" a forgotten woman chemist. Often, a name was mentioned in a correspondence or listed as a publication co-author which gave us the new avenue of research. One example was our "discovery" of the contributions of Polish researcher in radioactivity, Stephanie Horowitz (47), which began from a brief mention in a letter from Otto Hönigschmidt to Lise Meitner (48): "… Miss Horovitz and I worked like coolies. On this beautiful Sunday we are still sitting in the laboratory at 6 o'clock."

But are there many women chemists left to research? From our own experience, the answer is "yes." As a starting point, for the 19th century, Mary Creese produced an incredible four-volume sourcebook of women scientists (49-52). Many of the individuals described therein are worthy of much more thorough research.

For the early 20th century, probably the most fruitful source of "forgotten" women chemists is that of women-friendly research groups, for example, Frederick Gowland Hopkins at the University of Cambridge (44); Martha Whiteley at Imperial College, London (53); Lafayette Mendel at Yale (54); and Julius Stieglitz at the University of Chicago (55). Many of the American women chemists obtained their first degrees at U.S. women's colleges (55); likewise, British women chemists most often graduated from U.K. women's colleges (56), making women's college archives a fruitful source of names. Also, many women chemists were recruited for synthesis and research laboratories in the First World War (57).

There is much searching yet to be done. More pioneering women chemists to be discovered. Many more contributions to chemistry to be found.

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Marelene Rayner-Canham and Geoff Rayner-Canham have undertaken extensive research on the history of women in chemistry. In addition to authoring many publications, their most recent books are: *A Chemical Passion: The Forgotten Story of Chemistry at British Independent Girls' Schools, 1820s-1930s* (Institute of Education Press) and *Pioneering British Women Chemists: Their Lives and Contributions* (World Scientific Publishing Co.). Geoff is also the author of *The Periodic Table: Past, Present, and Future* (World Scientific Publishing Co.).

"THE POOR SISTER"
COMING TO GRIPS WITH RECENT AND CONTEMPORARY CHEMISTRY (1)

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Abstract

In 2007 a reviewer wrote that "The history of 20th-century chemistry has been the poor sister of physics and biology." Regrettably, that judgment is still valid. This paper argues for the necessity of elevating the profile of recent and contemporary chemistry (defined as chemistry of the last 60 and 30 years, respectively) in the historical literature and proposes a mechanism for doing so. It requires confronting a variety of challenges: the various audiences for history of chemistry that differ in technical and historical sophistication; the diversity of authors, among them chemists, chemist-historians and historians of science studying history of chemistry; and the necessity for adopting new research techniques and relinquishing some traditional ones. By far, most history of recent chemistry is written by chemists and chemist-historians and is only accessible to those with sophisticated technical training. However, that is not the only constraint preventing it from reaching a wider circle of readers. This body of literature lacks the essential contextual sophistication necessary for its inclusion in history of science publications. To overcome these barriers, HIST and the Science History Institute will collaborate on a workshop at the SHI connecting chemist-historians and historians of science in order to establish a shared background, to negotiate about the topic, structure, research agenda, and scope of proposed projects, and to plan for publication, when appropriate.

Introduction

"The history of 20th-century chemistry has been the poor sister of physics and biology;" such was the judgment of historian Ana Simões in 2007 (2). Examination of the annual volumes of the *Isis Current Bibliography* for the last dozen years indicates that Simões' assertion still holds. This paper argues for the necessity of elevating the profile of recent and contemporary chemistry (defined as chemistry of the last 60 and 30 years, respectively) in the historical literature, lays out the obstacles impeding such an effort, and proposes a program for overcoming those obstacles.

Background

A convincing case for engaging with the history of recent science was articulated in 1997 by Thomas Söderqvist, who noted that "the bulk of scientific activity in world history has taken place since World War II," and that "recent technoscience involves a significant portion of women … and scientists from outside the traditional European-North-American core" (3). In Ref. 3 and in a successor volume published in 2006, chemistry received scant attention, substantiating Simões' claim (4). Peter Morris's 2007 assessment of whether "modern" chemistry would receive increased attention from historians of chemistry was not optimistic (5). Four years later, Morris was somewhat encouraged. Yet, after posing the question, "Does the history of recent science have a future?" he found it "hard to say if the subject is on the rise" (6). Morris and Jeffrey Seeman express concerns about the pursuit of history of recent chemistry elsewhere in this issue (7). (I have adopted Morris's definition of "Recent Chemistry" (60 years) and halved that to arrive at a definition of "Contemporary Chemistry." I use "Recent Chemistry" as a catchall term unless specifically discussing contemporary chemistry. Furthermore, the term "historians of chemistry" denotes anyone who writes about the subject, regardless of professional affiliation. Further subdivisions of this denotation are discussed in a later section.)

Numerous impediments have been claimed to make writing the history of recent chemistry problematic. I have listed and assessed some major ones below. The first two have received abundant attention and will be considered only briefly; the remainder will be discussed in greater detail:

- The type of archival resources on which historians traditionally depend are mostly absent.
- The technical content is new and difficult and is accompanied by novel and unfamiliar terminology.
- History of recent science employs methodologies, such as oral histories and interviews, rarely used by most historians of chemistry.
- The boundaries of chemistry are becoming ever more blurred, as chemists increasingly find work in areas that lack the word "chemistry" in their title. Carston Reinhardt recently described chemistry as a "field of knowledge, a toolbox, an approach *delocalized over* the physical and life sciences, industries, and engineering" (8).
- Within this delocalized domain there are few, if any, headline-grabbing topics of the type found in neighboring sciences, such as physics and biology, that could provide an obvious starting point for anyone beginning to write about recent chemistry (9, 10).

Confronting Obstacles

Historians of science have long been admonished to treat science on its own terms, without the benefits of "retrospective insight." That ideal is easily achieved with recent science because there are no later standards to apply. Yet some historians find recent science unfit for evaluation precisely because of the absence of such standards (11). And while most commentators concede the difficulty of the contents and terminology of recent science, it has been argued that studies of the more distant past have not been free of that problem (12).

Some historians are troubled by the centrality of interviews and oral histories in the history of recent science. They emphasize the variable reliability of interviewees' memories and their inevitable tendency to put themselves in the best possible light. Advocates of oral testimony respond that cross-checking interviews with written documents and the testimonies of other interviewees provide checks on these shortcomings. They further aver that it is naïve to believe written documents are free of self-aggrandizement. Furthermore, the spontaneity of interviews permits the expression of unmediated observations often absent from written documents (13). Fortunately for historians of chemistry, the Science History Institute (SHI) in Philadelphia has a large collection of oral histories from interviewees in numerous fields falling under the "chemistry" umbrella and conducts oral history workshops (14).

The quotation that begins this paper requires qualification; problems that seem uniquely characteristic of the history of chemistry may be more widespread. Angela Creager has pointed out that "The history of biology is often presented especially in classrooms as either the history of evolution or that of genetics—or both ... Rarely do the non-hereditary, non-transmutational aspects of the life sciences, whether endocrinology or ecology, take centre stage" (15). A similar complaint has come from historians of solid-state physics: "Solid state physics is … a large, heterogenous, messy field ... [l]acking the unifying features beloved of historians ... [and having] neither a single hypothesis or set of basic equations … nor a single spectacular and fundamental discovery" (16). These remarks demonstrate that writing recent history of science without relying on "Block Buster" topics is not a problem unique to chemistry.

Different Audiences, Divergent Histories. Can They Be Reconciled?

Historians of chemistry fall into distinct groups having different professional backgrounds and often engaging separate audiences. The primary professional allegiance of chemist-historians is to organizations where chemistry is taught and/or practiced, while professional historians of chemistry have been characterized as "'historian[s] of science' doing the history of chemistry."

I use "historians of science" to designate historians of chemistry who are not chemist-historians (17).

The existence of several audiences for history of chemistry, defined by their degree of technical competence, is characteristic of our field. As Morris pointed out a decade ago, chemists produce the majority of publications in history of chemistry. Indeed, chemists have long written book-length histories of chemistry for a variety of readers, many of which have covered aspects of recent chemistry (18). At present, essentially all coverage of history of contemporary chemistry and much writing about history of recent chemistry has been authored by chemists (including chemist-historians), and usually appears in technical journals. Those publications serve to celebrate chemistry as a discipline, showcasing exemplary investigations and valorizing those who achieve them. While appreciated within chemical circles, these works assume sophisticated technical knowledge and are thus opaque to readers outside those circles (19).

However, chemist-historians often can and do write for a wider audience that includes readers with only modest chemistry backgrounds. A great many of these authors, regardless of location, write for publications connected to the American Chemical Society, particularly the ACS Symposium Series and the *Bulletin for the History of Chemistry* (20, 21). The technical content on these varies considerably, especially in the *Bulletin*, and a sizeable portion of its articles are accessible at least in part to historians of science. Yet even when achieving a desirable balance of technical and non-technical content, these articles only occasionally incorporate the degree of contextual detail expected of publications in history of science journals (22). Yet if the history of recent chemistry is to become known beyond the chemistry community, publication in these journals will be indispensable.

While only a minority of chemist-historians have written for history of science journals, they are the preferred outlet for historians of science. These historians typically seek out the political, social, economic, and personal contexts that significantly shape the history of chemistry. Unfortunately, the limited technical expertise of most historians of science constrains them from working on recent chemistry (23).

Thus, we have two parallel tracks of scholarship separated by disciplinary constraints and cultural differences that limit communication, much less cooperation. For history of recent chemistry to approach something like parity with history of both recent biology and recent physics, it will need advocates who have a secure grasp of both the science and its setting. Individuals with both capabilities are rare, and there is an almost unimaginably large terrain to be covered. An alternative is facilitating collaboration between chemists and chemist-historians on one side and historians of science on the other. This path has its own difficulties (24). Nonetheless, it holds out the hope of drawing more participants into this urgent but seemingly overwhelming task.

A Proposal for Raising the Visibility of Recent History of Chemistry

Chemists and historians are socialized into professional cultures that differ sharply in their canons of evidence, argument, and presentation. It follows that merely bringing members of the two groups together with little shared background and guidance is unlikely to lead to fruitful collaboration. In fact, it can easily produce the opposite effect. Söderqvist points out that "When it comes to recent and contemporary science … scientists often find it difficult to acknowledge the need for specific historical skills," while "Historians have so little understanding of recent science and may exhibit such insensitivity to scientists' way of thinking and understanding science that they cannot achieve the necessary rapport" (25). Thus, collaboration between chemists and historians of science is a process that, in large part, must be *cultivated*. It will involve recruitment of participants; establishment of some shared background; negotiations about the topic, structure, research agenda, and scope of proposed projects, and plans for publication, if appropriate.

Who might participate and how might they be identified? On the chemistry side, one cannot expect chemists with active research programs to be available. However, retired chemists and academic chemists at institutions lacking facilities for laboratory-based research yet requiring faculty research activity are potential candidates. They could be reached by an advertisement in the *Bulletin* (26), by announcement in the SHI online publication, *Distillations* (27), and by a notice posted to the CHEM-HIST list (28). It would be very desirable to have a story on this initiative in *Chemical & Engineering News*. Those resources collectively might well be sufficient to capture the attention of most historians of science interested in the history of recent chemistry but daunted by the technical barrier (29).

The principal activity would be a workshop, several days in length, which would concern itself with research techniques—doing oral history, conducting archival research—and historiographic issues—the varieties of history of chemistry, the criteria for judging them. The Executive Committee of HIST has agreed to support such an initiative by promoting it and seeking out potential participants (30).

However, the proposed program must be hosted by an institution capable of supplying the ancillary services essential for its success. The SHI is an ideal venue, given its facilities and its mission, and it has agreed to assume that role (31). The process envisioned would have the workshop led by one or two historians of science, possibly with the assistance of a chemist-historian who had published in several types of journal. A list of topics might be circulated during the call for participants in part to encourage work on recent chemistry. And if we take seriously Reinhardt's characterization of chemistry as "an approach *delocalized over* the physical and life sciences, industries, and engineering," then we should contemplate increasing the number of collaborating investigators and their disciplinary backgrounds."

Afterword

In recognizing the reality of modern chemical practice, most chemists have abandoned the image of the lone investigator at the bench. Perhaps historians of chemistry should reconsider the image of the lone investigator in the archives (32).

Acknowledgement

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10. Drawing on Harry Collins, Steve Fuller has asserted that "the contemporary period is the *only* one about which the historian can reliably write, mainly because the scientists have not yet had an opportunity to forge canonical accounts of their exploits, which then function as myths obscuring any hope of getting at [what] really happened," S. Fuller, "Who's Afraid of the History of Contemporary Science?" in Ref. 3, pp 245-259 on 246 (italics in the original).
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19. Although written for an audience of chemists, the two dozen or so autobiographies of distinguished chemists in Jeffrey Seeman's *Profiles, Pathways, and Dreams* series, published by the ACS in the 1990s, contains much material of interest and is accessible to historians.

20. In 2017 the University of Florence began publishing *Substantia. An International Journal of the History of Chemistry*, https://riviste.fupress.net/index.php/subs/about (accessed 21 Sep 2021), which is open access. Although focused on chemistry, it accepts articles from a wide variety of disciplines that range from the highly technical to the historical and philosophical. Among technical journals, *Angewandte Chemie* (English version, *Angewandte Chemie International Edition*), is notable for its receptivity to historical submissions.

21. Also noteworthy is *Distillations*, the online successor to *Chemical Heritage* magazine, published by the SHI, which also provides podcasts. The intended audience is less sophisticated than and orders of magnitude larger than those for all the above-mentioned history of chemistry/science journals. Writing for a lay audience requires skills additional to those encompassed by this paper, an activity to which we pay less attention than it deserves.

22. P. J. T. Morris, "Musings from a Departing Editor on the 75th Anniversary of *Ambix*," *Ambix*, 2**012**, 59(3), 189-196 on 194-195.

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25. Ref. 3, p 10; Ref. 6 (Kragh), pp 115-119.

26. The editor of the *Bulletin* has offered to publish announcements of the initiative: Carmen Giunta, private communication, 21 February 2021.

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About the Author

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THE IMPORTANCE OF PLURALITY AND MUTUAL RESPECT IN THE PRACTICE OF THE HISTORY OF CHEMISTRY

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Abstract

This paper emphasizes the need for professional historians of chemistry, chemist-historians and chemists to respect each other's contributions in the development of the history of chemistry. We posit that only a wide diversity of contributions including both entirely extrinsic and entirely intrinsic scholarship, and everything in between, will result in a complete history of chemistry. We also call for more scholarship in the history of modern chemistry and for the inclusion of history of chemistry in all chemistry courses. Several other recommendations are also provided.

"Science without its history is like a man without memory" (1) — Colin Russell (1984).

Preface

In 1993 Frederic L. Holmes (Figure 1) wrote in the opening sentences of his essay (2) in the book (3) *Chemical Sciences in the Modern World*,

> The great externalist-internalist debate of the 1970s now appears outdated, not because the questions raised during its prime have been resolved but because most of us grew tired of contesting the issue. It has been relatively easy to retire from confrontation, because rival claims could be settled merely by partitioning the history of science into two sets of subproblems. Those who were attracted to studying external situations [professional historians] have found ample scope to do so, while those who preferred what were lumped together as internalist problems [chemist-historians and chemists] were also free to go their own way. A minority of eclectic historians have made efforts, generally applauded, to penetrate more than superficially across the perceived boundaries, but their exemplary studies have not been seen as resolving the issue.

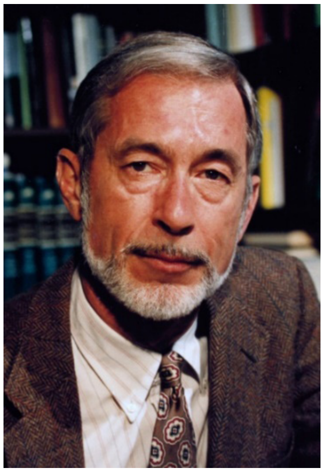

Figure 1. *Frederic Holmes. Photograph courtesy John Harley Warner and the Section of the History of Medicine, Yale School of Medicine.*

Holmes was prophetic. Historians do their thing (4, 5). And chemist-historians do their thing (6, 7). And a few "eclectic" scholars find some degree of synergistic bridging to their endeavors (8, 9). The barriers separating these two legitimate academies, silos in modern terms, have been reinforced by decades of organizational and behavioral norms. True, books and publications are published for all to read and use. But even a limited citation analysis (10) demonstrates that the intellectual territories poorly overlap, notwithstanding the skepticism of some (11) and support by others (12) regarding these concepts.

We, the authors, a professional historian and a chemist-historian, believe in the value of diversity and the importance of respect and even admiration amongst the practitioners of the history of chemistry (HoC). Where do these values take us in 2022 and beyond?

Introduction

This special issue of the *Bulletin for the History of Chemistry* celebrates the 100th Birthday of the Division of History of Chemistry (HIST) of the American Chemical Society (ACS). The theme for this special

Table 1. Chemists' and Chemist-Historians' versus Historians' Backgrounds and Research Activities

Topic	**Chemists writing "pure" chemistry**	**Chemists writing history of chemistry**	**Historians of science**
Undergraduate education	Chemistry		History and/or liberal arts and much less frequently science with some exceptions
Graduate education	Generally Ph.D. in chemistry		Ph.D. in history or history of science
Job position	Academic, government, industry, other		Department of History or Department of History of Science or retired from one of these positions
Time period of research in history of chemistry	Mostly post-1900		Mostly pre-1900
Number of publications and/or patents in a chemistry (sub) discipline	0 to over 100	Many, often over 50	Few or none
Collaborations within one's own discipline (intradisciplinary collaborations)	Many	Infrequent	Few to none
Participation in interdisciplinary collaborations	0 to many	Few	Few to none
Professional society memberships	ACS, RSC, and other national chemical societies	E.g., Division of History of Chemistry of the ACS; History Group of the RSC	SHAC, HSS, BSHS
Participation in professional society meetings	Yes	Yes, especially history of chemistry sections	History meetings
Reads their presentations	No		Yes
Browses chemistry journals at least several times/year	Yes		No
Browses history journals at least several times/year	No	Maybe to yes	Yes
University tenure criteria	Number of and quality of journal publications, funding		Number of and quality of books
Nature of academic practices	Science faculty have research groups with graduate students and postdoctoral students working closely with major professor		Faculty may mentor graduate students but not co-publish with them.
Associations with other departments	Not too often	Sometimes	Rarely

issue of the *Bulletin* is *Novel Insights in the History of Chemistry: Looking Back Yet Mostly Looking Forward*. To be responsive to this special issue's theme, we have, after much thought and several false starts, chosen the questions below as the central themes for our paper.

What is the history of chemistry? Who have contributed and will contribute to the HoC? What is the relationship between the various stakeholders in the HoC? Is the HoC maximally benefiting from the diversity of those active in the field? What is the future of the HoC?

There is an extensive literature on these issues. Over many decades, there have even been one major and several minor skirmishes in what might be called "the science wars" (1, 5, 7, 13-18). Even what constitutes the field of chemistry has grown and morphed (10). To maintain its own relevance, the American Chemical Society has enlarged its fleet of technical journals centered about one of its more recent titles, *ACS Central Science.* Following its merger with the Life Sciences Foundation in 2015, the Chemical Heritage Foundation changed its name in 2018 to the Science History Institute and, thereby, broadened its vision and mission.

In the meantime, the HoC marches on, following its own organic pathway. By "organic growth" we refer to an evolutionally natural process based on the activities and behaviors of members of the HoC community individually and spontaneously adapting to the situations at hand. In this paper, we intend to examine the pattern of growth and the health of the HoC endeavor as a function of its member-participants.

Discussion

The history of chemistry is the study of the development of chemistry. Over the last sixty years, HoC as done by chemist-historians and HoC as done by professional historians (also referred to as "historians" hereafter), have become separate academic fields. From a sociology of science perspective, chemist-historians and historians of chemistry inhabit different disciplinary silos characterized by their own unique behavioral norms. A listing of the most relevant normative behaviors of chemists, chemist-historians, and historians is shown in Table 1.

Importantly, the authors of this paper themselves reside rather firmly in these different silos, Morris being a historian and Seeman a chemist-historian. That this paper represents the best thoughts of each author and of the combined authorship team is noteworthy. One reviewer of this article wrote, "The authors clearly favor the chemist-historian/chemist type of history of chemistry over that of the professional historians." Certainly, the present authors have our own idiosyncratic professional stories. Yet we state unequivocally our equal support and admiration for all scholars who study and write the HoC. We strongly reject the conclusion of this reviewer.

There are some scholars who have maintained one foot in each camp, but they are few. Historian Alan Rocke (see Figure 2) is one; he has published papers in several chemistry venues (19-22) and is a Fellow of the American Chemical Society. On the other side of the coin is Steve Weininger, a recently retired academic chemist, who has published multiple times in history journals: three times in *Ambix* (23-25) and once in *Annals in Science* (26).

Figure 2. *(Left) Alan Rocke. (Right) Stephen Weininger. Photographs courtesy Cristine Rom and S. Weininger.*

All academic fields have their normative behaviors. Examination of Table 1 is particularly instructive, especially noting which behaviors are the same (just a few) and which different when comparing the chemist-historian silo with the historian silo. Many of these behaviors derive from one's academic training, in this instance, from one's undergraduate and graduate school experiences as well as the academic norms of one's professional institutions. For example, chemists obtain university tenure by publishing in high quality chemistry journals and obtaining major research funding. Historians usually obtain university tenure by having at least one book by respected academic publishers.

Clearly, the chemist-historians' norms *versus* the professional historians' norms are quite different. Chemists and chemist-historians unreflectively and unreflexively tend to follow the conventions of chemistry whereas historians follow their silo's conventions. The normative behaviors for both professions must be followed, else publishers, journal editors, and reviewers will reject their submissions and their careers will suffer.

Largely because of these conventions and the consequent skill sets of the individuals, HoC written by chemists is different from that written by historians (Table 2). Chemists have been writing the history of chemistry from the 18th century (1) though they have only been called chemist-historians in the last 60 years or so. The basis of chemist-historians' normative behaviors when writing HoC stems directly from their education as chemists. To see this, compare the normative behaviors of chemists with those of chemist-historians in Table 1, columns 2 *versus* 3.

Table 2. Chemist-Historians' Publications versus Historians' Publications

Topic	**Chemist-historians**	**Historians of Science**
Journals published in	*Bulletin for the History of Chemistry* and a few mainstream chemistry journals, e.g., *Angewandte Chemie*, *Nature Chemistry*	*Ambix*, *Isis*, *Annals of Science*, *Studies in History and Philosophy of Science*
Readership for publications	chemists	historians
Primary format for publications	journals	books
Co-authorships	infrequent	rare
Time-period covered	vast majority post-1900	generally pre-1900, mostly even pre-1850
Focus of paper	chemical developments (internalist) "typically focus on ideas and their sequential developments" (27)	social context of change (externalist) "typically seek to understand the relationship between scientific practices, scientific institutions and the wider society in which they exist" (27)
Treatment of historical events	"emphasis on heroic achievements of 'great men' and the linear development of theory" (27)	"less deterministic, more open-ended account of scientific development" (27)
Reliance on primary actors	Yes	Usually
Use of primary literature	Major	Minor
Use of secondary literature	Minor	Major
Style of publication	concise, scientific style	discursive
Use of problematization	no	frequent
Use of scientific data	Yes, especially post-1820s	Rarely ever
Inclusion of conclusion section	mostly, often extensive	rare and tend to be short
Use of chemical structures and reactions	Yes	Generally no
Similarity to chemistry publications	Yes	No
Similarity to non-scientific history publications	No	Yes
Use of substantive footnotes	limited, generally discouraged	common
Publishers' policy toward chemical formulae, chemical structures and reaction schemes	It is the publishers' standard practice to include structures in chemistry journals favored by chemist-historians	History journals generally do not encourage the publication of chemical structures

Though historians have existed for hundreds of years, historians of science as a profession first began in the 1930s. However, the history of chemistry was dominated by chemist-historians until the early 1960s. Thus, the two kinds of HoC have diverged from the first appearance of the scholarship of historians over those last sixty years. A watershed moment in the identification and specification of the norms of professional historians occurred about the time James Riddick (J. R.) Partington (Figure 3) wrote his massive four-volume series of the HoC. Historians rejected the kind of "history" that Partington and his fellow chemist-historians wrote. For example, noted historian and founding president of the Chemical Heritage Foundation Arnold Thackray (Figure 3) wrote of Partington's fourth volume and Aaron Ihde's *The Development of Modern Chemistry* (17)

Figure 3. *(Left) J. R. Partington. Photograph courtesy William B. Jensen and the Oesper Collections in the History of Chemistry, University of Cincinnati. (Right) Arnold Thackray, Smith Library, University of Pennsylvania, early 1970s. Photograph courtesy A. Thackray.*

> How much greater therefore one's disappointment that these works, though scholarly and authoritative, fail to appreciate or reflect the new climate of historical scholarship. Instead they remain firmly embedded in the old, and by now weary, tradition of chemical history by chemists for chemists. … A history of chemistry which does justice to the present insights of philosophers and general historians remains to be written.

What chemists write today is often in the same style as their predecessors wrote in the 1950s with a few exceptions. They emphasize the science, not the context. And that seems to meet the needs of their audience, mostly other chemists (and other chemist-historians).

Historians writing the HoC followed in Thackray's footsteps in challenging the traditional HoC model. Some of those challenges were empathetic, for example Stephen G. Brush's argument that (5)

> Scientists should write history of science if they are willing to acquire the skills and background knowledge of the historian of science … In this enterprise, those scientists who are willing to learn historical methods and study original sources have a continuing and essential role to play.

Thus, two silos started to form, one being chemists writing traditional HoC and the other being professional historians writing a new social HoC. It should not be thought that one silo contained chemists and the other historians with no chemical background. Many of the early professional historians of chemistry had undergraduate chemistry degrees, for example, William H. Brock, Maurice Crosland, Owen Hannaway, Colin A. Russell, Bill Smeaton, and Thackray. Their relationships with chemistry varied. Some strongly rejected the chemist's view of the HoC (e.g., Thackray (17)), others were proud of their chemical background but did not seek to retain links with chemistry (e.g., Brock (28) but see a recent collaboration with a chemist-historian (29)), and yet others positively strove to maintain the link between history and chemistry. A good example of the third group is Russell (30) (Figure 4), about whom his friend, Alec Campbell, wrote (31)

> The fact that the [RSC Historical] Group now has an established place in the programme of the Annual Congress, alongside the large Divisions of the R.S.C., is due to Colin's detailed knowledge of the interplay of forces within the history of science in this country, and his personal commitment to the notion of the history of chemistry as an integral part of living chemistry.

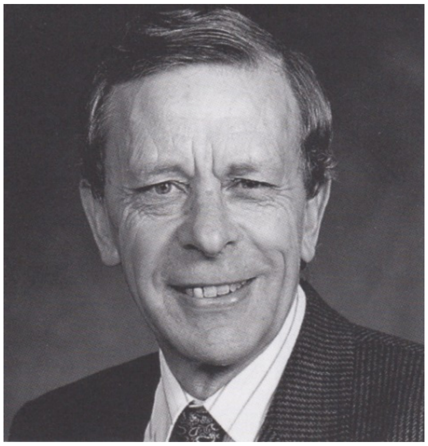

Figure 4*. Colin Russell, ca. 1985.*

The issue now arose, should chemists when writing HoC adopt the conventions and concerns of professional historians as stated by Thackray (17) and Brush (4, 5) among others? "*Ambix* is a history journal," Rocke stated to one of the present authors (JIS) during his tenure as Associate Editor of *Ambix*. Most historians have demonstrated by their actions that they prefer to publish in history journals, not journals read by chemists and chemist-historians.

In the 1980s and 1990s there were sustained efforts by historians to encourage chemist-historians to write the kind of history approved by historians. This was partly because some former chemists, especially Russell, did not want their fellow chemists to be viewed negatively, especially in the eyes of professional historians of science or the editors of history of science journals. There were various attempts at that time to get chemists to "buck up" and write the "proper" history of chemistry, notably in a book review (32), paper (33), and essay (34) by one of the present authors (PJTM). The Center for the History of Chemistry also tried to get chemists to adopt the professional historians' norms after the Center was founded in 1982. The hand of its founding director Thackray was surely behind this influence, for example, in holding a conference *Chemical Sciences in the Modern World* for historians and chemists at the Eagle Lodge Conference Centre outside Philadelphia in May 1990. A comprehensive book (3) edited by Seymour Mauskopf is one lasting consequence of that meeting, notable in part for documenting the concerns of historians of chemistry some 30 years ago.

In contrast, there was strong support for the inclusion of chemistry in HoC studies and in chemistry textbooks (35). One of the most strongly worded statements about how chemists should write HoC was penned by the historian with the strongest chemical background (a former lecturer in chemistry with several chemistry research papers to his credit (36)) and the one most anxious to retain the link of professional history with professional chemistry, namely Russell. He wrote (1)

> At a conference some years ago to celebrate the bicentenary of an important British scientist, papers were planned about his literary work, his reforming ideals, his public lectures, his institutional affiliations—even his sporting life! Only as an afterthought was anything proposed concerning his science, though that was the single reason for his importance. Instances like this can be multiplied. They arise when a rightful concern with the context of science has been extended to an almost monomaniac obsession, to the virtual exclusion of its content.

There were also attempts in the 1990s and 2000s to bring chemist-historians and professional historians together in conferences. These meetings engendered a degree of interest and good-will on both sides, but eventually chemists ceased to come to meetings which were under the control of professional historians and mostly geared to their intellectual outlook. Historians often participated in meetings organized by HIST but chemists rarely attend history conferences. For all of us, financial costs and time availability are serious constraints in attending multiple meetings per year.

The Science Wars of the 1990s largely passed the chemist-historian silo by, although Jay Labinger and Harry Collins co-edited an eirenic book *The One Culture? A Conversation about Science* (37). However, the Science Wars may have increased the wariness of some chemist-historians towards the agenda of the historians and their intentions regarding chemist-historians. This rejection of the historians' approach was partly pragmatic: the customers for the publications of chemist-historians were other chemists who expected adherence to their own conventions and approach to developments in chemistry.

In terms of journals and publishers, it is an undeniable fact that the journals patronized by professional historians gear their style of publications to an academic professional historian audience which embraces the same style of research and writing. At present, chemist-historians have several publication venues available to them, such as several journals dedicated to the HoC including the *Bulletin for the History of Chemistry*, the British RSC Historical Group *Newsletter*, the German *Mitteilungen der Fachgruppe Geschichte der Chemie* and the Japanese *Kagakushi*. Chemist-historians and chemists have also published HoC in several chemistry journals, such as *Angewandte Chemie, Chemistry—A European Journal, The Chemical Record*, and on one-off occasions, *The Journal of Organic Chemistry* (38, 39) and other journals of the ACS (40).

Neither silo is about to disappear. We should appeal for mutual understanding and respect between the members of the two silos for their own style and content of their version of HoC. The professional historians should cease to judge the published output of the chemist-historians by their own criteria—criteria it has to be said were at least partly introduced in the 1960s and 1970s to demarcate the new "professional history of chemistry" from the older more traditional HoC. At the same time, chemist-historians should accept that professional historians are making valid criticisms of the norms of chemist-historians, that context does matter, and that chemist-historians should consider adding more context to their research content. And in the same spirit, professional historians should add more science in their research and in their publications. It is hoped that the application of these ideas may lead to more interdisciplinary collaborations such as the recent publication by Brock and David Lewis (29) or texts such that *Chemical Sciences in the 20th Century: Bridging Boundaries* (41) edited by the historian and former president of the Chemical Heritage Foundation, Carsten Reinhardt.

We do not expect or wish the two silos to merge. That would be unrealistic and would even be detrimental to the field of HoC. In the same way that different fields of science collaborate in interdisciplinary research, we would hope that a growing number of chemist-historians and professional historians will feel able and encouraged to collaborate. Precisely by recognizing and validating the qualities of each silo, we anticipate the participants can seize unique interdisciplinary opportunities and achieve greater academic synergies.

We and certainly others have a growing concern about the study and documentation of the history of recent chemistry (42). There are relatively few chemist-historians or historians writing the history of recent chemistry (chemistry after 1970, a period of no less than 50 years!). Few books and publications on the history of recent chemistry exist other than those written by chemists and chemist-historians written in the style most appreciated by chemists. One of the present authors (PJTM) noted in 2011 that chemist-historians traditionally had taken their histories of chemistry up to the present (33). However, this revival, if it ever existed, has seemingly petered out. On the other hand, Morris was the editor of a volume on the cultural history of chemistry which, at the publisher's request, went up to 2019 (43). And chemist-historian Noboru Hirota has recently published a *History of Modern Chemistry* (44) which goes up to the 21st century. Hirota has more technical detail than the volume edited by Morris, but they are both very general works and are no substitute for a sustained account of the recent history of chemistry.

Writing the recent history of chemistry has several challenges. To understand recent chemistry, one needs at least some advanced level of chemical education. Yet relatively few professional historians of chemistry now have a chemistry background and fewer chemists are writing about that era of HoC. The volume of scientific papers being published is growing exponentially and it is also becoming interdisciplinary. Fifty years ago, it was possible for one chemist to understand practically all of chemistry and to make generalizations about it. This is no longer the case.

Furthermore, as historian Brush noted 25 years ago (5),

> Scientists have much to contribute to the history of science, and there are certain kinds of important questions that can be discussed only by those who have considerable technical background.

Historians find writing the history of today's modern chemistry challenging if not impossible. We speculate that, just as now, some established professional historians in the future will have begun their academic careers as chemistry students, and then shifted into history of science—although they are likely to be few. For these individuals and perhaps for others too, the corpus of modern chemistry is far beyond understanding for non-professional chemists. Who then can write about today's recent chemistry (and "recent chemistry" in the years to come)? Is the field left only to chemists and chemist-historians? If this becomes the case, then professional historians of chemistry will forever be locked into studying pre-1900 chemistry. Or if they venture beyond that era, they will do so by ignoring "certain kinds of important questions that can be discussed only by those who have considerable technical background" (5). One possible solution: interdisciplinary collaboration (7).

We now make a serious leap in terms of what we consider to be scholarship in the HoC. Who could really argue that the substance of discovery—the compounds, the reactions, the chemical and physical properties of matter, the actual achievements of chemists—is not a key component in the HoC? To do so would be not just unrealistic, but absurd. We posit that journals such as *Accounts of Chemical Research* and *Chemical Reviews* represent valid and necessary contributions to the HoC.

Figure 5 qualitatively illustrates our view as to the role of various publication media with regard to the HoC and the audiences they each serve. We first discuss the upper axis. At the left end of the scale (left and right are chosen arbitrarily) are journals that include HoC with a major if not sole emphasis on externalist factors. These are populated by history journals such as *Ambix* and *Isis*. At the right end of the scale are journals whose major if not sole emphasis is on internalist factors. These are populated by chemistry journals such as *Accounts of Chemical Research* and, at the far right, *Chemical Reviews*. In the middle are journals that include articles that bring both internalist and externalist perspectives in their articles. We posit that the journals cited at the far right in Figure 5 also contain information relevant to the HoC. The inclusion of *Accounts of Chemical Research* and *Chemical Reviews* as sources for the HoC may seem surprising to some historians as well as perhaps to some chemists.

We recognize that not all HoC is published in professional journals. The second axis in Figure 5 is somewhat orthogonal to the first axis in that it represents media for whom the primary readership is a more general population. The now on-line *Distillations* published by the Science History Institute is a blended publication in that its readership is primarily science professionals, yet the articles are written such that a more general population will also be properly served.

We first analyze the upper axis in Figure 5. At a simplistic level, look just at articles that appear in history of chemistry journals. There is hardly a single chemical pictograph of a molecule, a reaction, or a reaction mechanism in most *Ambix* articles. Let us consider an *Ambix* paper written by a chemist-historian that is more likely to have internalist material when compared to *Ambix* articles written by historians. Chemist-historian Weininger's recent 25-page *Ambix* article entitled "Delayed Reaction: The Tardy Embrace of Physical Organic Chemistry by the German Organic Community" contains pictography of one reaction and two sets of structures (two pairs of resonance hybrids) (25). Even though he is a chemist-historian, Weininger's text is mostly about externalist factors affecting the course of chemistry in Germany in the 20th century and skirts around what the science of physical organic chemistry was in the 20th century. In contrast, papers in *Accounts of Chemical Research* or *Chemical Reviews* contain page after page of chemical structures, reactions and mechanisms. Our claim is that we need both, articles in *Chemical Reviews* as well as articles in *Ambix,* to fully appreciate and characterize the HoC.

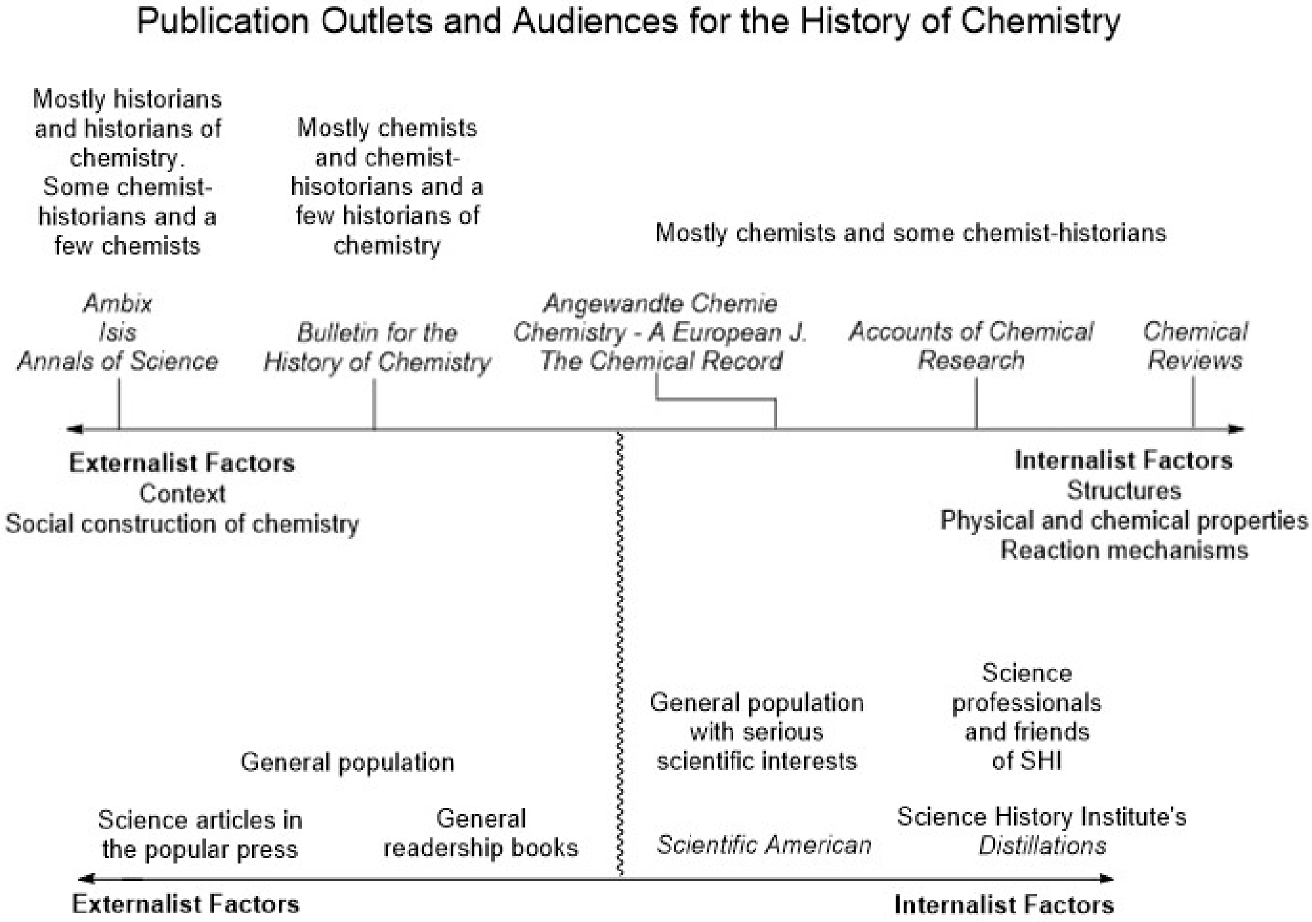

Figure 5. *Illustration of the qualitative relationships between chemical content and contextual content of HoC and various publication media. The positions on the two axes are not drawn to scale, and the location of the somewhat orthogonal general population media denoted by the wavy line is arbitrarily placed. The history of chemistry is a discipline that contains both externalist and internalist factors.*

We believe that historian Rocke got it exactly right when he wrote in 2018 (45),

> If one wants to gain greater clarity on what happened in chemistry, one needs to focus not just on what our historical protagonists *say* and *write*, which is surely important enough, but also on what they *do*, and even on what we might conclude about what and how they *think.* They experiment, pay attention to empirical details, and think about the results of others; they use innumerable instrumental methods to probe the unseen; … they manipulate formulas on paper, build physical models ….

Unfortunately, primary documents for research dealing with the late 20th century and thereafter are mostly unavailable and will continue to be so. Letters have been replaced by email (and increasingly so for other even more ephemeral media such as WhatsApp or Snapchat); neither telephone calls nor Zoom meetings are typically recorded and preserved; and laboratory notebooks are being replaced by computer files or purely electronic data. Hence, if current "data" germane to the HoC is not captured and archived while its originators are still alive, it will not available for future historians of chemistry (46, 47). Ironically, archivists would prefer documents in electronic format, as they are inexpensive to store and relatively easy to search. But that requires chemists to save and donate their electronic files including their emails, an unlikely proposition given that they may contain personal material or material the scientists consider confidential—exactly the material that those studying the HoC would desire!

On the issue of personnel to write this recent history of chemistry, by 2000, there were fewer chemically-trained students *entering* the professional history of chemistry field, and more were and are being drawn from English and history disciplines. There were even fewer full-blown Ph.D. chemists entering this field with a Ph.D. in history or history of science, notwithstanding certain exceptions such as Lawrence Principe at Johns Hopkins and Catherine Jackson at Oxford. The interests of the history professionals were also shifting from the 19th century and the Chemical Revolution to the early modern period (16th to early 18th centuries) and alchemy and chymistry. This meant that the field of 20th-century chemistry was being increasingly abandoned to the chemist-historians. It appears clear today that only chemist-historians will have both the interest and the technical understanding to comprehensively cover this field. That said, this field does offer possibilities for interdisciplinary research, with the chemist dealing with the technical details and the historian producing the contextual aspects. But does the history community, including and especially their tenure committees, reward interdisciplinary research as does the chemistry community? We believe not.

There appears to be a growth in the number of chemists who are interested in the HoC, not just to read HoC but to produce HoC research, though often on a one-time basis to satisfy a particular motivation. These individuals might be called hobbyists, as one of the present authors thought of himself for several decades (JIS). So how are more chemist-historians recruited, in general, and recruited specifically to work on the recent history of chemistry? Conferences and workshops could be instituted to encourage chemists to study the history of recent chemistry, an idea that might be attractive to those who are on the brink of or past retirement. Even if chemists only wrote about their own life's work, or that of their Ph.D. advisors, in an intelligent, self-aware manner, this would be an important source of information on the recent history of chemistry. There is a major precedent for this in one of the present author's (JIS's) *Profiles, Pathways and Dreams* series of autobiography. Another such source are the biographical memoirs written about the deceased Fellows of the Royal Society (London) and members of the United States National Academy of Sciences (NAS). The authors of the memoirs of chemists are almost always chemists. For example, the organic chemists John D. Roberts and Lord (Alexander) Todd (Figure 6) authored eight biographical memoirs for the NAS and six for the Royal Society, respectively.

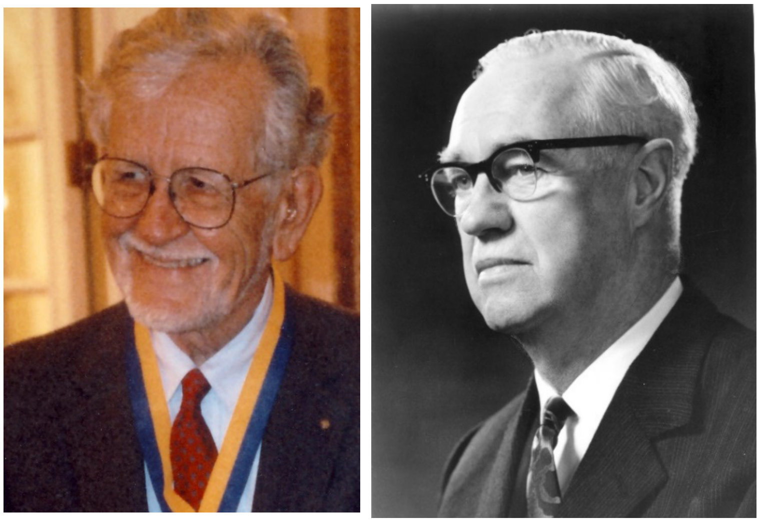

Figure 6. *(Left) John D. Roberts and (Right) Lord Todd. Roberts photograph courtesy J. I. Seeman. Todd photograph courtesy the Royal Society (London).*

We encourage the editors and publishers of all journals—both history of science journals and chemistry journals—to be more welcoming to cross-disciplinary authored submissions. These would include manuscripts written in an author's cultural norm which may be quite different from that journal's norms and its readership's expectations. At the same time, authors must always be sensitive to a journal's standards and its own culture. It is surely unrealistic for a journal to publish a paper whose content and style are many deviations outside its own norm.

We now focus on the lower axis of Figure 5. Authors of articles that appear in *Distillations* or in *Scientific American* understand that their readers are not necessarily science professionals. But authors for and editors of such media know that their readership has expectations for scientific content that exceeds the content that appears in newspaper articles and magazines such as *Time* and *People*.

Which brings us to Weininger's interesting proposal in his article in this special issue of the Bulletin (42). Weininger believes that the HoC published by chemists and historian-chemists "lacks the essential contextual sophistication necessary for its inclusion in history of science publications" (42). But this conclusion may not consider the needs and requirements of the journal, the authors, and the readers of the articles to which he refers. The articles written by the chemists and chemist-historians referred to by Weininger may contain, likely do contain the exact right blend of context and substance for their specific situations, as shown in Figure 5. In the same vein, the articles that appear in the history journal *Ambix* may contain the exact amount of scientific detail as needed by the publisher, editors, authors and readers of that journal.

Weininger's proposal, to have a workshop co-sponsored by HIST and SHI, "to overcome" (42) the insufficiencies in the articles written by chemists and chemist-historians are particularly likely to succeed if those authors intend to publish in journals like *Ambix* which are history journals. As we discussed in Tables 1 and 2, the cultures of chemists and of historians are so very different that, to meet the goals of crossing disciplinary boundaries, authors can truly benefit from instruction by those in their sister discipline. This conclusion goes equally well for historians who wish to publish in chemistry or chemistry-oriented journals. On the other hand, as we recommend in the next section, perhaps journals and editors ought to be more welcoming to cross-disciplinary submissions. Diversity is a good thing! All this being said, more HoC context in chemistry articles and more chemistry in history articles may be a good thing all around.

Finally, we make an appeal for the return of the history of chemistry in chemistry courses. While we are perfectly aware of the pressures on the chemistry syllabus, we believe that a discipline that does not know its history cannot learn from its past errors. There is an inevitable tension about whether such courses should be taught by chemist-historians or professional historians. This is essentially a false choice. Historians will demand too much independence in their modes of instruction from their academic institutions. Chemists will claim they have the capability to include HoC in their courses but have neither the time nor the resources and perhaps not even the inclination to do so. The academic chemists would also claim that the necessary course content does not permit the addition of HoC to the syllabus. We can envision that organizations such as the Science History Institute and HoC societies, mindful of the above stated limitations, could develop supplementary material that would make HoC available easily and free to instructors and students. Certainly, the HoC material that might be used in the classroom is very much a matter of an institution's educational requirements and the instructor's taste, and a "one size to fit all" approach would not find much use.

Conclusions

We conclude:

- Chemistry, as a discipline, is strengthened by a well-documented and easily available scholarship of its entire history.
- The practice of the history of chemistry is and will be determined "organically," influenced by societal factors, e.g., financial support for academic departments incorporating the history of science, the presence of history of chemistry journals and also high-quality chemistry journals that publish articles on the history of chemistry, the presence of leading book publishers in the history of chemistry, etc.
- There are two major silos of scholars studying the history of chemistry: professional historians, i.e., individuals whose advanced degrees are in history or history of science though some may have educational backgrounds in chemistry; and chemist-historians, i.e., individuals whose

advanced degrees are in chemistry or the molecular sciences. Individual chemists at times produce one or several publications in the history of chemistry, though they do not consider themselves chemist-historians.

- Historians write primarily for other historians. Chemists and chemist-historians write primarily for other chemists and other chemist-historians.
- As Mary Jo Nye has observed (48), there are many storylines in which the HoC can be told.
- We posit that journals like *Chemical Reviews* and *Accounts of Chemical Research* contribute to the total sum of knowledge in the HoC.
- Today, professional historians of chemistry are typically writing about pre-1900 chemistry and increasingly about pre-1800 chemistry and alchemy.
- Today, chemist-historians are generally writing about the period between 1870 and 1980.
- Chemists and chemist-historians are the most able and the most willing to write the history of recent chemistry.
- Nonetheless, insofar as the history of recent chemistry is being produced primarily by chemists and chemist-historians, the lack of historians studying recent chemistry suggests that the field is in danger of being insufficiently served.
- Research and publications in the history of chemistry will benefit from the widest diversity of scholarship and contributors to the field. We join others (49) and conclude that the contributions from *all* scholars in the HoC bring together *in toto* the scholarship that is called "the history of chemistry."

We offer the following recommendations:

- The history of chemistry for any era must include the social and organizational aspects of the chemistry (externalist) as well as the chemistry (internalist). To write a complete history of chemistry for any era likely will require the contributions from scholars having diverse knowledge and experiences.
- Regardless of one's disciplinary silo, all information should be used in the compilation of the history of chemistry, in general, and in the study of any one topic, in particular.
- Individuals in each silo should respect the styles, language, and cultures of others and especially value the academic production of their interdisciplinary colleagues.
- Efforts to force a bridging of these two silos have failed in the past and are probably doomed to fail in the future. Rather, interactions between individual scholars and the societies to which they belong should be encouraged but not with a "missionary vision." The two silos should take their own routes. They are two unique disciplines with little in common except they share the same historical data (the same scientists, the same scientific results, the same context, and so forth).
- Chemists and chemist-historians should be mindful of including externalist content in their papers, as appropriate for the intended journal and its readership. Historians should equally be mindful of including internalist content to their papers with the same caveats.
- Journal editors and reviewers of chemistry review articles should encourage authors to include more HoC in their papers. Editors should also commission more chemist-historians, and even historians, to write reviews.
- Chemists and chemist-historians (as well as historians) benefit from rigorous peer review of their manuscripts. A diversity of peer reviewers should be engaged by journal editors, a process that will provide for "organic" or "natural" improvement and growth in scholarship.
- Active and recently retired chemists should be encouraged to assist in studying the history of chemistry, especially the recent history of chemistry.
- The inclusion of a blend of internalist and externalist history of chemistry within chemistry courses at both the undergraduate and graduate level is rare and should be enhanced. Institutes focused on the history of science can provide a professional level of context-oriented supporting material for all educational levels.

We also are realists. We recognize that some of our recommendations may be rejected by professional historians and/or chemist-historians. We may be whistling in the wind. But remarkably, and certainly most happily, the present authors have discovered during the course of several years of dialogue and several months of writing this paper that we have each moved our positions much closer toward the other. Even if that is the only benefit of this manuscript, we are pleased. But we also are optimists. If we can expand our visions and feel gratified, so can others. Organically. For the benefit of all.

Coda

From an anonymous reviewer: “Let a hundred flowers bloom, and let’s all read each other’s work, I say!”

Dedication

This paper is dedicated to William B. Jensen, founding editor of the *Bulletin* and a notable chemist-historian and recipient of the 2005 Edelstein Award for Lifetime Achievement in the History of Chemistry.

Acknowledgments

The authors thank Carmen Giunta for the invitation to participate in this special issue of the *Bulletin* and Giunta, Bill Brock, Mary Virginia Orna, Alan Rocke, and two anonymous reviewers for very helpful comments and suggestions. We also thank Steve Weininger for allowing us access to his paper (42) prior to its publication.

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About the Authors

Peter J. T. Morris received his B.A. in chemistry from Oxford University and his undergraduate dissertation (Part II) was on *The Education of British Chemists in the Eighteenth Century.* He received a D.Phil. from the Faculty of Modern History at Oxford for a dissertation on the development of synthetic rubber at IG Farben. After a postdoctoral fellowship in the history of chemistry research group at the Open University, Milton Keynes (with Russell), he was an Assistant Director (Projects) at the Center for the History of Chemistry at the University of Pennsylvania (with Thackray) for three years. Subsequently, he was at the Open University as the first Royal Society-British Academy Research Fellow in the History of Science. In 1991, he was appointed Senior Curator in Experimental Chemistry at the Science Museum London, and then became Manager of Research in the Collections Unit of the Science Museum before ending his career at the museum as Keeper of Research Projects.

Jeffrey I. Seeman received his B.S. in chemistry from Stevens Institute of Technology, Hoboken, New Jersey, and his Ph.D. in chemistry from the University of California, Berkeley. He was a research chemist for over 30 years in industry and a fulltime consultant in the field of chemistry for another 10 years. In 1983, Seeman published his first paper in the history of chemistry (50). His first career highlight in HoC was the creation and editing of a 20-volume set of autobiographies of eminent organic chemists entitled *Profiles, Pathways and Dreams* which was published by the ACS from 1990 to 1997. In 2007, Seeman accepted a courtesy appointment in the Department of Chemistry at the University of Richmond in his hometown in Virginia. As his work in chemical research decreased in magnitude in the early 2000s, his research in the HoC correspondingly increased to the extent that today it consumes most of his professional time.

European Society for the History of Science

In 2022, the European Society for the History of Science (ESHS) will host its tenth biannual conference. This year's edition will take place in Brussels, Belgium, and is organised by the National Committee for Logic, History and Philosophy of Science (NCLHPS) of Belgium.

The theme of the ESHS 2022 conference will be Science Policy and the Politics of Science, a topic with a particular resonance over these past years. The outbreak of Covid-19 has called attention to the shifting legitimacy of science-based expertise and the reliance on expert authority in policy-making by state and national governments. Clearly, this serves as an indication for a need to understand the role of scientists and scholars in society within a broader historical frame.

Proposals on all periods, geographic locations, and areas of specialization are welcomed, addressing topics including, but not limited to, the following:

- Institutions, places, and spaces of scientific knowledge: centre and peripheries
- Patronage and science funding: public and private interests
- Theory and practice in scientific and technical expertise
- Material, visual, and textual cultures in the institutionalization of the sciences
- Circulation and networks of scientific knowledge
- Colonial histories and heritage in the sciences
- Gender and ethnicity in scientific institutions and leadership
- Trials and standardization in science making
- Openness and secrecy in the dissemination of scientific knowledge
- Amateur scholarship, lay practice, and citizen science
- Trust and authority in scientific discourse and policy
- Scientific movements, ideologies, and related historiographical narratives

To submit paper proposals, send the filled-in template (available at the website) as an attached file by email with subject line: "ESHS 2022 Paper Proposal" to eshsbrussels@gmail.com. The deadline for paper proposals is 21 February 2022, 23:59 CET.

Further information can be found at https://eshsbrussels2022.com.

THE LONG AND SHORT OF IT: THE FUTURE WRITING OF HISTORIES OF CHEMISTRY

William H. Brock, Hon. Research Fellow, Department of Science and Technology Studies, UCL, UK; william.brock@btinternet.com

Abstract

Following reflections on the experience of writing a long, thick history of chemistry in 1992 and, some 24 years later, a short thin one in 2016, the author notes how quickly the historiography of chemistry changed in just two decades. He asks whether book-length histories of chemistry, whether long or short, have a future. While the writing of biographical articles may seem straightforward, journal articles present problems as contemporary chemistry becomes more and more bound up with its sister sciences, computing and engineering, and the history of science with social and cultural history. Probably the only way to tackle late twentieth- and twenty-first-century chemistry satisfactorily is through a collaboration between technically-trained chemists and historians of science who may (or may not) have studied chemistry in their early education. The author reflects on two of his recent experiences of such collaboration.

Introduction

One of the sources I once used to understand how the Oxo Company manufactured Liebig's Extract of Meat was an article in one of the beautifully illustrated, four volumes of *Chemistry in Commerce* (1). Evidently published in weekly parts, the volumes covered a wide range of industries that were active in the 1930s, ranging from electroplating to gas manufacture, brewing and the manufacture of pharmaceuticals. It was particularly good on the food industry. What struck me in perusing the pages was that all of the dozens of analytical quality control procedures mentioned and illustrated in the volumes were all time-consuming wet analyses. The only instrumental techniques mentioned were pyrometry, the design and use of autoclaves, and one brief essay on an automatic recording device. From the present perspective, there was also a complete absence of information on the monitoring of waste products of industry and on pollution and its control.

As historians and chemists well know, the sea change in analytical instrumentation occurred in the 1950s (2). The second edition (1951) of Arthur Vogel's *Quantitative Inorganic Analysis*, which I used as an undergraduate in 1956, still emphasized the need for the classical training in group analysis laid down as student exercises by Liebig in the 1830s at the University of Giessen (3). Instrumentation was arriving while I was a student, but it was slow in affecting British undergraduate training, mainly because electronic instruments were still beyond the financial resources of the average College laboratory. Vogel's textbook did, in fact, have chapters and illustrations of instruments for calorimetry, potentiometry and polarography, but my undergraduate generation was never introduced to them. I do not recall handling any instrument, other than an ordinary spectroscope, until my third and final year when, while investigating the spectra of tetrahedral molecules, I was allowed to use the department's one and only spectrophotometer (4).

The point of these personal reflections is that any historian, like myself, who abandoned chemistry sixty years ago, is severely disadvantaged by lack of experience with instrumental investigations involving IR or UV spectroscopy, mass spectroscopy, gas chromatography and NMR, let alone production control instruments in industrial settings. Inevitably, then, those of us who retrained as historians of science in the 1950s and 1960s have tended to investigate chemistry's deeper past, particularly the development of alchemy (if we have Latin), the early modern chemistry that is now appropriately dubbed chymistry, the eighteenth-century chemical revolution, the establishment of atomic theory, and the emergence of organic chemistry, valence and structural formulas at the end of the nineteenth century. But we remain ill-equipped to deal with twentieth-century chemistry, let alone the chemistry of the recent past.

Today, most of the younger generation of historians of science have taken degrees in the humanities which may, or may not, have included some history of science, but they have not studied the physical sciences beyond school level. Few have had practical experience in the laboratory. Consequently, they face a problem when dealing with twentieth-century and more recent chemistry beyond writing about it from a sociological perspective.

A Long, Thick History

I wrote most of my *Norton History of Chemistry* in 1990-91 at the Chemical Heritage Foundation (now Science History Institute) in Philadelphia. It was published in the UK in 1992 and in the States a year later, as part of a series of volumes planned by the late Roy Porter to embrace the whole of the history of science and culture. Sadly, for various reasons, volumes on the history of physics and biology never appeared. When I returned to the States in the summer of 1993, I learned that my book was a "bestseller" and was being recommended by the *New York Times* (5). The work is now nearly thirty years old and, in several respects, out of date. Like chemistry itself, historical interests and perspectives change and evolve. The historiography of the subject has, not surprisingly, greatly altered since 1992, notably with changed perspectives on the role of alchemy, the significance of Robert Boyle, the role of synthetic methods in the development of structural chemistry in the nineteenth century. The book also lacked a place for a full treatment of physical chemistry. Despite decent sales and its use in undergraduate teaching, a revised edition was never called for. Although the book carried no overt "message," by being arranged around what might be considered as defining "landmark" monographs and papers from Lucretius's *On the Nature of the Universe* to Ronald Nyholm's "Renaissance of Inorganic Chemistry," I was able to tell chemical stories around each of these "landmark" items that avoided the drudgery of chronology; it was intended to appeal to a readership of both professional chemists, general readers and, of course, historians of science. Oddly, around the same time, several other historians of chemistry published their own "take" on the subject (6), leading the late George B. Kauffman to express amazement at such a plethora of books by professional historians of science "when courses were no longer a part of the usual undergraduate curriculum." He compared his own introduction to the discipline in Claude Deicher's class at the University of Pennsylvania in 1950 when the only suitable text was by the chemist Frank J. Moore (7).

Chemists have always needed to be aware of the historical background to their research. This was the purpose of finding aids, such as those provided by Berzelius, Gmelin and Beilstein, or patent lists. These reference works provided information on who had first made compounds x and y, how they were prepared, and in what journals background papers and information might be sought (8). Abstracting services and annual reviews of the literature by diverse chemical societies followed at the beginning of the twentieth century. Complementing such aids to research were the long or short histories that chemists such as Thomas Thomson, Hermann Kopp, and many others have published since the beginning of the nineteenth century (9).

With no new edition of my "history" being called for, when, in 2013, Oxford University Press invited me to write a history of chemistry for its attractively-illustrated and inexpensive series of "Very Short Introductions," I leaped at the opportunity (10, Figure 1). The OUP pocket-size series was first launched in 1995 as accessible ways to find about a whole range of subjects new to a reader. The series now extends to over 600 books and includes, apart from my own contribution, 35.000-word monographs on the history of astronomy (M. A. Hoskin, 2003), mathematics (J. Stedall, 2012), medicine (W. B. Bynum, 2008), the periodic table (E. Scerri, 2011; 2nd ed. 2019), physics (J. Heilbron, 2018), the Scientific Revolution (L. M. Principe, 2011), as well as fine introductions to chemistry (P. Atkins, 2015), organic chemistry (G. Patrick, 2017), and physical chemistry (P. Atkins, 2014). In addition, there have been biographies of Bohr (J. Heilbron, 2020), Copernicus (O. Gingerich, 2016), Darwin (J. Howard, 2001), Faraday (F. A. J. L. James, 2010), Galileo (S. Drake, 2001), and Newton (R. Iliffe, 2007). Together, and with others still to follow, the books make an excellent introduction to many aspects of the history of the sciences (11).

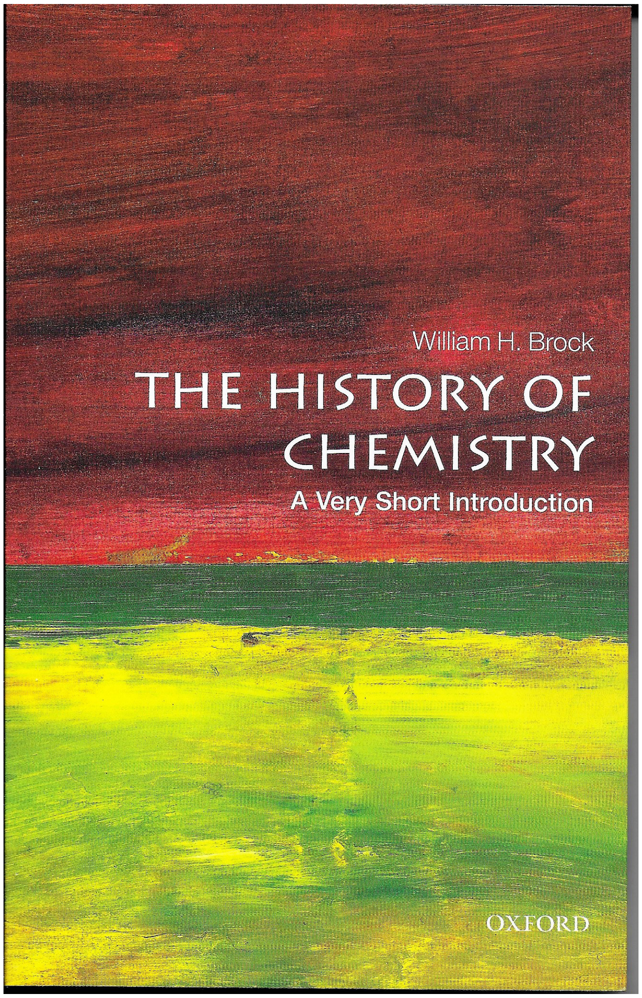


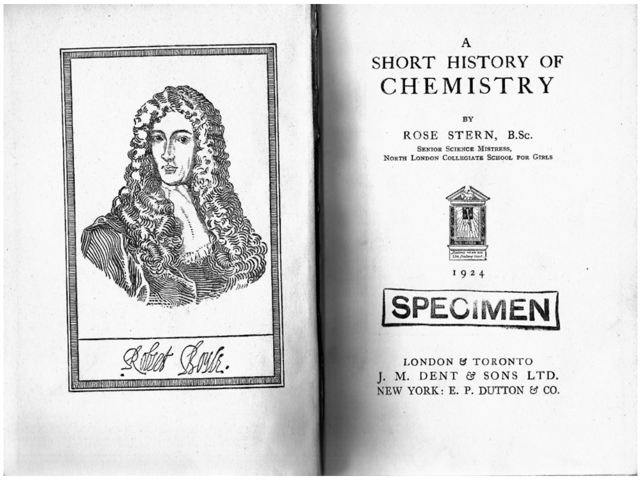
***Figure 1**. William Brock's history of chemistry entry in Oxford University Press's "A Very Short Introduction" series, bearing a cover typical of the series. Reproduced courtesy of OUP.*

Short Histories

Most authors in the series, myself included, have divided their word limit into six chapters of 5000 words apiece, allowing another 5000 words for overrun, preliminaries, bibliography and index. But some have opted for short chapters of 2,000 words. In opting for six chapters, I wondered whether any historian of chemistry had limited themselves in such a way before, apart from writing an encyclopedia entry—which OUP warned against. A literature search soon showed that there had been several volumes entitled *Short History of Chemistry*, beginning with Francis Preston Venable, a German-trained chemist at the University of North Carolina who published his book in 1894. Although only 183 pages in length, it seems most likely that he called it "short" in comparison with Hermann Kopp's 4-volume German history (1843-47) each volume of which was roughly 400 pages in length (12). Venable's book was based upon lectures he gave to chemistry undergraduates in the belief that history added to their understanding of modern chemistry. It was divided into six chapters, Genesis, Alchemy, Qualitative era (Paracelsus to phlogiston), Quantitative (Dalton and Berzelius), Structural Chemistry and Periodicity (one of Venable's specialties), and a final chapter on Specialization.

Ignoring William Tilden's "short history" of 1899 which only covered recent progress in the chemistry (13), the next chemist to compile a short English text was Thomas Percy Hilditch (1886-1965). This was frankly a pot-boiler written when he was a post-doctoral student working with William Ramsay at University College London in 1911 (14). It was designed for undergraduates to pass a University of London compulsory paper on the history of chemistry—an examination paper that formed part of the B.Sc. degree until the end of World War II. This explains the call for several reprints as late as 1922. Hilditch called his book "A Concise History" rather than a short history, presumably because he tabulated much of the information. It was certainly concise, but it was not short, running to 263 pages. It is not without merit since it still offers today's historian a wide view of the state of chemistry in the early 1900s, especially organic chemistry. Hilditch never returned to history. In 1911, he entered the soap industry of Joseph Crosfield in Warrington just when the firm was being absorbed into the alkali company of Brunner Mond. In 1925 he was appointed to a chair of industrial chemistry at the University of Liverpool from where he wrote many hefty books on the chemistry of natural fats.

Secondary school science teachers also needed information on the history of chemistry because chemistry was often taught from an historical perspective, especially when demonstrating and teaching about gases and combustion. Rose Stern (1869-1953), who had studied chemistry with Percy Frankland at the University of Birmingham (B.Sc. 1894), taught chemistry at a leading London girls' school, the North London Collegiate. She encouraged many of her pupils to take up chemical careers, as the Rayner-Canhams have noted (15). In retirement, in 1924, she published a short history for schoolgirls as well as other science teachers (Figure 2). Interestingly, she ended the story in 1900 because she thought more recent work on radioactivity and atomic structure was too difficult for young minds (16).


Robert Boyle.

A
SHORT HISTORY OF
CHEMISTRY

BY
ROSE STERN, B.Sc.
Senior Science Mistress,
North London Collegiate School for Girls

1924

SPECIMEN

LONDON & TORONTO
J. M. DENT & SONS LTD.
NEW YORK: E. P. DUTTON & CO.

***Figure 2**. Rose Stern's title page and frontispiece, 1924. Reproduced under Fair Dealing exemption.*

Eric J. Holmyard (1891-1959) was another, more famous, schoolteacher at the important private school, Clifton College, Bristol, that has often been noted for producing alumni who took up scientific careers and who often became Fellows of the Royal Society (17). Holmyard, who taught both physics and chemistry from an historical viewpoint, was also a significant self-taught Arabist and one of the founders of the Society for the History of Alchemy and Early Chemistry in 1935 (18). His books *Chemistry to the Time of Dalton* (1925), *Great Chemists* (1929) and *The Makers of Chemistry* (1931), although not entitled "short," should also be included in the discussion (19). Meanwhile, Holmyard's physical chemistry contemporary, James Riddick Partington, whose work needs no introduction to the *Bulletin's* readers, produced his short history in 1937. In retrospect, it can be seen as the ground plan for the multi-volume history of chemistry that he planned to occupy his retirement and to be the English "Kopp" (20).

Short histories continued to be produced after World War II. Isaac Asimov was commissioned to write one (Figure 3) for the post-*Sputnik* American Science Study education series, that also included I. B. Cohen's magnificent *Birth of the New Physics* explaining Newtonian dynamics (21). Asimov was a professional biochemist in New York who wrote many popular science books. His short history was not a bad book, but its purpose was help High School youngsters learn chemistry through the medium of its history and not to offer fine analysis and detail. And finally, and most recently, we have the French work by Sacha Tomic, a pupil of Bernadette Bensaude-Vincent (herself the co-author of a previously mentioned history of chemistry and a work on the philosophy of chemistry) that very much reflects on the Janus-faced nature of chemistry and the need for a greener industrial chemistry in the twenty-first century (22).

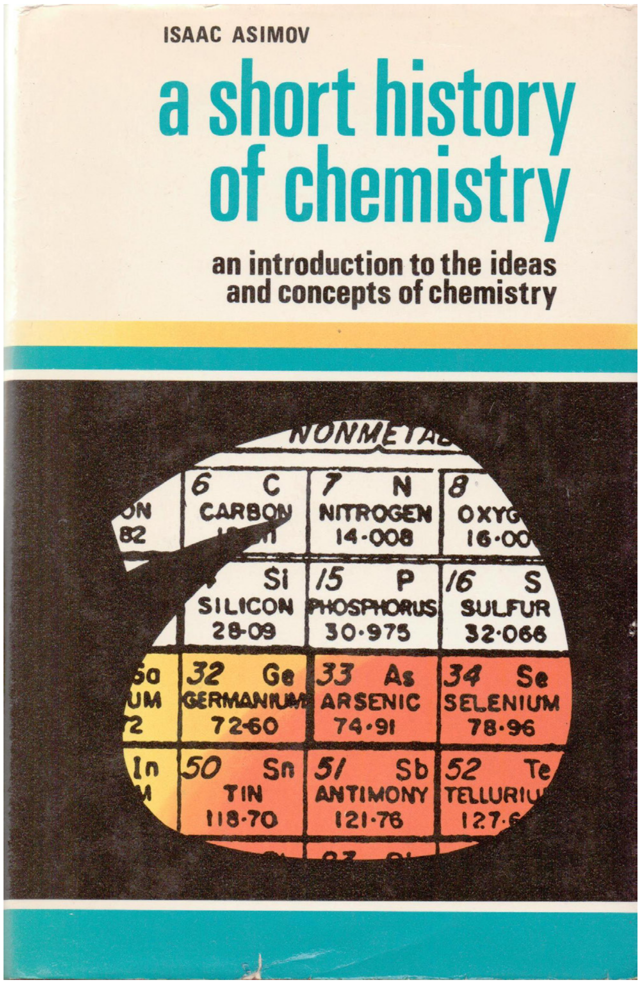

ISAAC ASIMOV
a short history of chemistry
an introduction to the ideas and concepts of chemistry

***Figure 3**. The first edition of Asimov's short history, 1965. Reproduced courtesy of Penguin Random House.*

This literary and bibliographical investigation revealed to me that there were many historical models for writing short histories. Most had been written for school/college/university educational purposes and not for historians *per se* or the general reader. The aim of OUP's series was to attract readers who were not just academic historians of science, but an educated public that included chemists and anyone curious to know what chemists have done in the past and what its developmental landmarks were. Constrained to 35,000 words, what should be included? What could be left out? Industrial chemistry, that deserved its own short history, was an obvious candidate for just a fleeting mention. Otherwise, I decided to build a narrative around the theme that chemistry is the science of change, metamorphosis and transformation of matter, and how its historiography had altered since the 1990s.

How the Historiography has Changed since 1992

The result was, probably in many readers' eye, a fairly conventional narrative beginning with the changes wrought in historians' minds by archaeological chemistry and the modern instruments of analysis that have enriched our views of ancient technology. I was particularly intrigued that the still was probably evolved from the hearths originally used in cooking and early metallurgy. Alongside this, there was Marco Beretta's work on glass as an artisanal craft that began in Egypt and had a close connection with alchemy through the coloring of glass to make artificial jewelry. The glass theme coupled nicely with the recent work of Catherine Jackson and her argument that useful synthesis only began in Germany in the 1870s when chemists found the ability to blow their own specialized apparatus and to adopt new safety measures in laboratory design (23).

There had also been a completely new interpretation of alchemy produced by the researches of William R. Newman and Lawrence M. Principe that undermined the old debate as to whether alchemy evolved into chemistry or whether it had offered nothing to modern chemistry except raw data about acids, alkalis and salts, as well as useful bits of apparatus. We can now see chymistry (with a y) as a respectable artisanal occupation whose members were applied chemists and chemical engineers who applied their skills for powerful European patrons. Some, but not all, believed in the possibility of metallic transmutation, but this never lessened their employability. Alongside this we have to face Andrew Cunningham's argument that the world picture of early modern European scholars was totally different from that which followed in the eighteenth-century Enlightenment and the naming of "the scientist" in the 1830s (24). Their observations and experiments were conducted in a world in which macrocosm and microcosm, and the entailed linkages between man, nature and God, were literally a world apart from the world of Lavoisier and Dalton. There is a discontinuity in the history of the sciences that has to be confronted when writing about early-modern chemistry. Older histories often christened Robert Boyle as "the father of chemistry," but our understanding of Boyle has matured following his placement in the context of his contemporaries like George Starkey and Daniel Sennert, while Michael Hunter has explored his voluminous archive (25). The work of various scholars has clarified the reasons for Boyle's (and for that matter, Newton's) deep interest in alchemy, and thereby illuminated the details of his corpuscular, but non-mechanical philosophy, and its links with the ancient ideas of atomic *minima.*

For the eighteenth century, Jonathan Simon's work on the pharmaceutics tradition has highlighted the hitherto much neglected, but real, importance of the development of French chemistry via the extraction of salts from plants that led to the fundamental chemical theorem that acids + bases = salts (26). The theorem led to affinity tables and the evident tension between theories of matter that were physical in orientation (like Boyle's) and chemical by way of property-bearing principles (like Stahl's). Lavoisier, too, has to be seen anew, in terms that stress his reformation of chemical language and nomenclature and another crisis of tension between physics and chemistry evidenced in the work of Priestley. Hasok Chang in his *Is Water* H_2O*?* has also challenged historians by asking what was lost when phlogiston was abandoned (27). He notes that important chemical problems disappeared from view—problems that were only resolved many decades after phlogiston vanished. He highlights the character of metallicity that was explained by phlogiston, but only "explained" in the twentieth century by electrons. His intriguing idea of scientists and historians engaging in "complementary science"—that is, looking at past experiments that got nowhere, deserves the attention of chemists and historians of chemistry.

Structural chemistry has also received a new lease of life for historians. Debates over the significance of Liebig's potash bulbs have been crowned by work on glass and its significance for organic chemists in creating apparatus that helped in determining structure by degradation and synthesis at the end of the nineteenth century. Finally, there has been an astonishing growth in the philosophy of chemistry since 1990, and a new appreciation of how twentieth-century chemistry transformed the world through a combination of academic chemistry and chemical engineering, and new black-boxed instruments and computers that replaced painstaking wet and dry methods of chemical analysis—the starting point of this essay.

The Future

What then of the future of history of chemistry? Do book-length histories of chemistry, whether long or short, have a future? The recent appearance of a multi-volume history of chemistry in German, and the forthcoming multi-volume cultural history of chemistry, suggests the answer is undoubtedly affirmative (28). But I believe "short" accounts are the most promising way forward, either as articles or as monographs. In fact, the genre of "short" monographs on specific topics in the history of chemistry had been established by the Scottish chemist Andrew N. Meldrum as far back as 1904, but was not followed up by later chemists (29). While the writing of biographical articles may seem more straightforward, journal articles present problems as contemporary chemistry becomes more and more bound up with its sister sciences, computing and engineering, and the history of science with social and cultural history. Probably the only way to tackle late twentieth- and twenty-first-century chemistry satisfactorily is through a collaboration between technically-trained chemists and historians of science who may (or may not) have studied chemistry in their early education.

Bearing in mind, and with tongue in cheek, that "collaboration" can also mean "cooperation with the enemy," we should recall and overcome William Jensen's exploration of "the problematic relation" between contemporary historians of science and the interests of professional chemists (30). In practice, my own recent experiences of collaborating with professional scientists, who are interested in the history of their science, has worked remarkably well (31). It has, however, revealed a minor issue involving the very different presentation styles expected by editors of scientific and humanities journals. Academic humanities periodicals always expect authors to cite the full titles of cited literature, where science journals only ever require the citation of the relevant journal's title (in a standardized abbreviated form such as suggested by CASSI), the volume number and the article's first page number; titles are ignored. Consequently, because the actual titles of twentieth-century and contemporary chemistry articles can be interminable (particularly if they form part of a series of investigations), the cumulative effect is the production of a very long paper. The length is further increased because the expectation—indeed, the requirement—of history of science editors and their referees is that there should be the fullest possible reference to the existing secondary literature relevant to the topic. A paper for an historical journal can thereby easily exceed the length tolerance of the periodical concerned. A compromise will need to be found—a formula already suggested by *Angewandte Chemie, Chemistry—A European Journal,* and *Substantia*—for articles on historical topics. Another solution is the one followed by Meldrum in the early twentieth century, namely short monographs that explore thematic topics, a facility now happily provided by the SpringerBriefs mentioned in Alan J. Rocke's essay in this issue (32)—though, curiously, such a collaboration between chemist historian and historian of chemistry has yet to appear in the series.

There is much to do. Such future collaborative ventures might exploit the many rich European and American archives that have been deposited by chemical practitioners, explore chemists' relations with the professional societies and publishers; create more histories of important teaching and research departments; highlight less well-known chemists such as Frederick Abel or Frank Dainton, who played significant roles in government. My files bulge with potential topics that, as an octogenarian, I am unlikely ever to have the chance to explore: accounts of chemists who spent parts of their careers in the colonies of various nations, particularly in India and Australia; explorations of chemical feuds, and of blind alleys (or alternative chemistries) such as the claims of the spectroscopist Cyril Baly that he had carried out photosynthesis *in vitro*, or of the not unimportant pre-electronic Barlow-Pope model of crystallization.

Conclusion

While there will continue to be ample scope for further interpretations of the progress of chemistry before 1900, there is an even greater need for interpretations of the history of chemistry since then. (See the essays in this volume by Stephen Weininger and by Peter Morris and Jeffrey Seeman for further thoughts about the history of recent chemistry (33).) The way forward, I suggest, is through journal or monographic collaboration between chemical historians (or professional chemists) and historians of chemistry. This is not a new idea and there are already some exemplary models. But it is the only way forward given the complexity of contemporary chemistry and that the majority of historians of science have received no training or research experience in chemistry. The history of chemistry will always be an important and valuable adjunct to the study of chemistry. As Liebig wrote to his former pupil and sometime agricultural antagonist, Joseph Henry Gilbert, in 1870 when he declined an invitation to deliver that year's Chemical Society Faraday Lecture, he had been studying the history of chemistry and recalling how he regretted giving up his friendship with Berzelius over thirty years before (34):

> I have learnt that all our theories are not Truth itself, but resting places or stages on the way to the conquest of Truth, and that we must be contented to have obtained for the strivers after Truth such a resting place which, if it is on a mountain, permits us to view the provinces already won and those still to be conquered.

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About the Author

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DOES HISTORY OF CHEMISTRY HAVE A FUTURE?

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Abstract

Brief remarks are offered on the current status and future prospects of the following topics, mainly in the United States: historical resources for the history of chemistry; textbooks and history of chemistry courses; history of chemistry and general chemistry; organizations and journals for history of chemistry; chemical historians and historians of science. Because history is not a predictive science, this is more an opinion piece than a documented piece of history.

When I first volunteered a contribution with the above title, I did so because I thought it was a perfect fit for the theme of this special issue of the *Bulletin*. Only later did I realize the full repercussions of what I had done. While Mark Twain's famous quip that "history does not repeat itself, but it often rhymes" has a certain vague, albeit amusing, truth to it, the grim reality, as repeatedly emphasized by Karl Popper, is that history is not a predictive science (1).

An historian, by definition, deals with the past and not with the future. He traffics in factual evidence, even though his personal biases may color both his choice of that evidence and his interpretation of its significance. This means that, in choosing the above subject for my contribution, I have removed myself from the realm of proper history and instead placed myself among those psychics whose annual predictions of the future clutter the pages of the *National Enquirer* and other such dreadful publications found in the checkout aisle of your local grocery store. In keeping with this, what follows should be viewed more as an opinion piece or editorial than as a properly documented contribution to history.

Over the years several of my previous publications have obliquely touched on aspects of the above topic and this is especially the case with a paper I presented as part of a symposium organized by Sy Mauskopf in 1993 (2-4). What I intend in the following is to update my comments found in these earlier papers. I will first briefly review the current status of the following topics: historical resources for the history of chemistry; textbooks and history of chemistry courses; history of chemistry and general chemistry; organizations and journals for history of chemistry; chemical historians and historians of science, followed in each case by my opinion of their future prospects. For obvious reasons I will deal largely with the situation in the United States, since I have more direct personal knowledge of this.

Historical Resources

Current Status

By historical resources I mean significant collections of period books, chemical journals, prints, photos and physical artifacts of interest to the chemical historian. I will say nothing about such primary sources as personal papers, diaries, company or institutional records, etc., since it is not possible to make generalizations concerning either the locations or accessibility of such materials (5).

Books and Chemical Journals: Collections of books and chemical journals of interest to chemical historians are available at the Oesper Collections in Cincinnati, Ohio, the Science History Institute (formerly the Chemical Heritage Foundation) in Philadelphia, Pennsylvania, and the Edgar Fahs Smith Collection at the University of Pennsylvania (6). In all three cases their holdings span the 20th century back through at least the 17th, if not earlier. Typical examples of other, smaller, but significant collections include the Morgan Collection in the History of Chemistry at Ohio University in Athens, Ohio (7), the History of Science Collections at the Linda Hall Library in Kansas City, Missouri, and the Williams Miles Textbook Collection in the History of Chemistry at Harding University in Searcy, Arkansas. For those specializing in alchemy, there is the Ethan Allen Hitchcock Alchemy Collection at the St Louis Mercantile Library in St Louis, Missouri. Unlike the case of the Oesper Collections, several of the above collections are not housed apart but are rather submerged within larger, more generalized, library holdings.

Prints and Photos: Once again large collections of both prints and photos relating to the history of chemistry are to be found in the Oesper Collections, the Science History Institute, and the Edgar Fahs Smith Collection. The Frank B. Dains Print and Portrait Collection, which was used extensively to illustrate Mary Elvira Weeks' classic study, *Discovery of the Elements,* is to be found in the library collections at the University of Kansas in Lawrence, Kansas. On the other hand, the Ferris Jewett Moore Collection of Chemical Portraits at MIT, which was the basis of the 1949 book by Smith (8), has apparently disappeared (9). There are also several sites on the internet which attempt to sell scans of historical prints and photos relating to the history of science, despite the fact that the images in question have long been in the public domain.

Artifacts: Every major American city has either a science museum or a natural history museum or both. However. neither of these institutions deals with the history of science, let alone with the history of chemistry. To be blunt about it, both, to an increasing extent, are currently focused on entertaining children—the former via interactive displays for them to play with, and the latter via extensive displays centered around that favorite of all small boys—the dinosaur, both as fossil skeletons and increasingly as life-size animated mechanical models. Nor are we talking about the traditional 19th-century chemical museums that were often associated with university chemistry departments and which consisted of displays of important chemical products. The best known of these in the United States were those created by the brothers, William and Charles Chandler—the first at Lehigh University and the second at Columbia University (10-12).

There are, of course, many proper, albeit smaller, historical collections scattered throughout the United States that deal with either the history of medicine or the history of pharmacy—the latter usually in the form of a reconstructed 19th-century drug store. Though not their major focus, both kinds of collections often contain small amounts of 19th-century chemical apparatus (13). However, far more extensive collections of historical chemical apparatus may be seen in the reproduction of Thomas Edison's Menlo Park Laboratory at Greenfield Village in Dearborn, Michigan, and at his original laboratories in both West Orange, New Jersey and Fort Myers, Florida.

Harvard, Yale, MIT, Dartmouth (14), and Transylvania University in Lexington, Kentucky (15, 16) all have collections of historic scientific instruments, though most of their holdings deal with apparatus used to teach physics and astronomy. Years ago I was given a tour of the storerooms for the collections at Harvard and saw many items related to the history of chemistry, though none of them were on display in the museum itself. I suspect this is also true of the other historical instrument collections.

The reasons for this apparent avoidance of historical chemical apparatus are interesting. Unlike the beautiful brass and ivory 18th- and 19th-century self-contained instruments used to teach physics and astronomy, for which it is often possible to trace the instrument maker responsible for their creation, traditional bench-top chemical apparatus was, and still is, largely modular and anonymous. Take the simple case of distillation. Just displaying the separate pieces of glassware and hardware used to construct a typical distillation train would be both uninformative and boring. The pieces have meaning only when assembled to illustrate how they were actually used in the laboratory by practicing chemists. This requires period heat sources, stands, clamps, condensers, distillation flasks and/or retorts, adapters, receivers, and possibly fractionating columns, depending on how elaborate the setup. It is improbable that all of these parts would come from a single source, let alone be labeled with the company that originally made or sold them, and so there is no instrument maker to trace. In addition, minor but key parts are often missing, such as a cork, rubber tubing, or a bent glass tube. If a purist demands that these be period pieces as well, rather than modern substitutes, the proposed display will never see the light of day. In addition, pre-pyrex (i.e., 19th-century and earlier) glassware did not exactly have a long life expectancy and so it is often necessary to use modern reproductions instead.

Much larger general museums, such as the Smithsonian in Washington, DC, and the Deutsches Museum in Munich, also own large collections of historical chemical apparatus, only a fraction of which is on display. At one time the Deutsches museum featured displays of impressive reproductions of so-called alchemical laboratories and 16th-century distillation apparatus (17, 18), as well as a reproduction of Liebig's famous laboratory at Giessen. Likewise, the Smithsonian featured displays of Joseph Priestley's laboratory apparatus, and Ira Remsen's circa 1876 laboratory at Johns Hopkins in Baltimore.

Though there are many museums in Europe that specialize in historical chemical apparatus, such as the Daubeny Collection at Oxford (19) or the Liebig Museum in Giessen (20), the only two in the United States that I am aware of are, once again, the Oesper Collections in Cincinnati (21) and the Science History Institute in Philadelphia. To aid in the study of these artifacts, both of these locations also own large collections of apparatus catalogs spanning the 19th and early 20th centuries.

Future Prospects

In summary, there are abundant resources available to the chemical historian. Indeed, most of the above collections, as well as the many European and British collections I have not mentioned, can be located via their own internet sites. The book, print and photo collections absorbed by various libraries are most likely safe from future loss, though their direct use will increasingly decline as more and more of this material becomes available online. At most they risk being dispersed among the other books in these libraries instead of being concentrated in a special area, as appears to have been the fate of both the Morgen Collection at Ohio University and the Henry Carrington Bolton Portrait and Book Collection at the Library of Congress (22).

The same is true of the artifact collections found in national museums. Though safe from destruction, they risk being overwhelmed by the vast holdings of these institutions, if not completely relegated to the store rooms, as they respond to the increasing public demand for more and more entertaining displays for children. For this reason, I am uncertain whether the history of chemistry displays mentioned above for the Deutsches Museum and the Smithsonian are still there. Perhaps the worst example of this fate I am aware of involves the Liebig Museum in Giessen. Recent video posted on the internet shows school children watching a modern whizz-bang chemical demonstration show in Liebig's original lecture hall and video of the adjoining laboratory shows a nonsensical jumble of antique and modern apparatus on the central tables more characteristic of the set for a Frankenstein movie than of a realistic depiction of a circa 1850 working chemical laboratory.

The artifact collections most at risk are those connected with universities. Many times these are the creations of a single faculty member interested in history of science. However, once that faculty member retires, the chemistry or physics departments involved are often unwilling to hire a replacement. When coupled with the usual academic squabbles over funding and space, the final result is dispersal, since librarians are not comfortable dealing with physical artifacts rather than books. Such was apparently the fate of the Moore Portrait Collection at MIT, and illustrates the wisdom of Arnold Thackray when he severed the connection between the original Center for the History of Chemistry and the University of Pennsylvania.

Textbooks and History of Chemistry Courses

Current Status

In my 1993 contribution to the Mauskopf volume, I was able to cite only one survey of colleges and universities that were offering a course in the history of chemistry, and the results were not promising (2). This is in large part because such courses are seldom part of the required curriculum for chemistry majors, but rather rely on an interested faculty member willing to offer such a course as an elective. History of chemistry courses are almost as rare within history of science departments, but for a different reason that I will mention in the later section dealing with the interactions between chemical historians and historians of science.

Unhappily, the American Chemical Society (ACS) has played a significant role in undercutting history of chemistry courses. When I formed my own course at the University of Cincinnati, as required by my endowed professorship in history of chemistry, I asked that physical chemistry be listed as a prerequisite, since much of the history of late 19th- and early 20th-century chemistry dealt with its subject matter. According to the standards for an ACS certified degree, this meant that the course qualified as an advanced chemistry credit. When the ACS discovered this, they refused to certify the BS chemistry degree at Cincinnati until this requirement was removed. In the end, in order to populate the course, since our majors could no longer use it to fulfill part of their advanced credit requirements, I had to offer the course from 4:30-5:30 pm so I could attract high school chemistry teachers and industrial chemists after working hours. In the end I had more students from chemical engineering, pharmacy, and philosophy than I did from our chemistry department.

Needless to say, a history of chemistry course also requires a good history of chemistry textbook that is compact enough to use for what is normally a one semester course. Currently Dover Books has kept several 20th-century classics in print as relatively inexpensive paperbacks, including those by Leicester (23), Partington (24), and Ihde (25). Yet another example is the more recent history by Bill Brock (26).

Future Prospects

The situation with respect to history of chemistry courses is unlikely to change much in the future. They will continue to be elective and to rely on chemistry faculty with a personal interest in the history of chemistry to teach them. At worst, populating such courses with chemistry majors will become more and more of a challenge as the progress of modern chemistry and the resulting increase in ACS degree requirements fill up more and more of the curriculum. With the possible exception of the textbook by Ihde, most of the books mentioned above do a poor job of covering the history of chemistry after 1930, so there is always room for future textbooks that also deal with the last two thirds of the 20th century and possibly with the first two decades of the 21st century (3). This will be quite a challenge, if I am to judge by what has happened in the chemistry department at Cincinnati, and I suspect elsewhere. The traditional *quadrivium* of analytical, organic, inorganic, and physical chemistry is beginning to dissolve. Traditional wet analytical chemistry has essentially disappeared and been replaced by instrumental analysis (27); organic chemistry has mutated into biophysical chemistry and drug design; physical chemistry into computational chemistry; and inorganic chemistry into material science. These changes have been driven as much by shifting patterns in research funding as by the science itself. There is also the problem that many histories of chemistry show a definite national bias relative to the chemists who are featured.

These trends do not necessarily mean that future history of chemistry textbooks will necessarily be larger. It is just as probable that they will splinter into smaller specialist histories. This has long been the case with separate histories for both biochemistry (28) and industrial chemistry (29), and I am also currently aware of separate histories for such subjects as polymer chemistry (30) and clinical chemistry (31).

History of Chemistry and General Chemistry

Current Status

A related topic is the question of how much history of chemistry should be included in the typical introductory chemistry textbook, not to mention the further question of whether it is possible to write such textbooks from an exclusively historical point of view. There is a vast literature on this subject in the education journals. Actual attempts to implement such an approach go back at least as far as the 1950s and the *Harvard Case Histories in Experimental Science*, edited by the American chemist, James Bryant Conant (32), and I think there were even earlier attempts at the University of Chicago. Most of these experiments focused on the use of history of science in college-level general science courses for nonscience majors, though they always contained a chemistry component.

As far as actual chemistry textbooks go, the impact of these approaches has been virtually nil. The only true example of an exclusively historical approach to general chemistry I am aware of is the 1915 textbook by Thomas Lowry, which I have described in detail elsewhere (4). Since at least 1910 the usual claim that your typical chemistry textbook has taken history into account means that there are photographs of famous chemists interleaved throughout the text, each with a two-sentence biographical summary. However, the motives for this are not historical but rather because—according to the publishers—they "humanize" the text. Like textbooks for the history of chemistry, these photo selections often show a distinct national bias.

Future Prospects

I strongly doubt whether the current situation will change in the future. An introductory textbook based on history of chemistry would never be tolerated by your average chemistry department. Indeed, once again the ACS is a determining factor in all of this. Years ago

Mary Virginia Orna served on an ACS committee tasked with developing an introductory chemistry course for nonscience majors. She suggested using an historical approach that I had outlined in a series of articles published in the *Journal of Chemical Education* (33). As she later told me, the committee refused to even consider the possibility of such an approach.

Organizations and Journals for History of Chemistry

Current Status

The ACS Division for the History of Chemistry (HIST) was founded in 1921 and as such is the oldest known professional organization for the study of history of chemistry, with the possible exception of the now defunct Alembic Club (34). From 1948-1967 HIST published an annual, single-volume, hard-cover journal called *Chymia*, and since 1988 has published the *Bulletin for the History of Chemistry*. The second oldest organization for the study of history of chemistry is the British Society for the Study of Alchemy and Early Chemistry, now Society for the History of Alchemy and Chemistry, which dates from 1935, and which began publication of its journal, *Ambix,* the next year (35). Though there are currently several additional organizations and journals for the study of history of chemistry, such as those in Germany and Japan, both *Ambix*, the *Bulletin* and their attendant organizations remain the most important for English speaking chemists and historians.

Future Prospects

As long as there are chemists interested in the history of their science, these organizations will continue to survive. Whether the changes brought on by the COVID pandemic will lead to the increasing use of remote rather than actual physical meetings of these organizations is extremely doubtful since everyone knows that the primary function of these meetings is social networking rather than as a necessary means for presenting original research that in most cases will also appear in print. Likewise with the journals published by these organizations, though these suffer a greater risk of eventually disappearing as hard copy and instead becoming internet publications only. As an old curmudgeon, I hope this will not happen, since I still delight in holding an actual physical copy of a book or journal in my hands rather than viewing it on a computer screen.

Chemical Historians and Historians of Science

Current Status

In recent years it has become common to differentiate between chemical historians (also called chemist historians elsewhere in this issue), on the one hand, and historians of chemistry, on the other, where the former refers to chemists interested in history and the latter to historians interested in chemistry. Chemical historians are by definition self-taught amateurs when it comes to history, whereas many historians of chemistry are self-taught amateurs when it comes to chemistry.

These differences are also apparent in the kinds of books and articles they write. Specialist histories of chemistry written by chemical historians, like those mentioned earlier by Morawetz on polymer chemistry (30) or Rosenfeld on clinical chemistry (31), tend to present each advance in theory or technique in great detail, complete with any necessary equations or chemical formulas, whereas those written by historians of science tend to focus on the sociological aspects of a given discipline, such as the development and politics behind the founding of the requisite professional organizations and journals or the internal squabbles between various key figures (36).

As I have commented in a recent book review, historians of science tend to avoid chemical formulas and mathematical equations as much as possible, apparently for fear their inclusion will damage sales of their books with regard to general readers (37). This is naive to say the least, since I doubt very much that such academic tomes have much of an audience among the general public, their primary readers being either other historians or interested chemists. To attempt to write about the history of a science while simultaneously refusing to use the language of that science is ludicrous in the extreme .

Since at least the 1980s HIST has made an effort to include professional historians as invited speakers whenever it has sponsored special symposia. Likewise, professional historians have long been comfortable publishing articles and reviewing books in *Ambix.* More recently the same is also true to an increasing extent for the *Bulletin*, especially under the current editorship of Carmen Giunta. Unhappily, there is little or no reciprocity. Chemical historians are seldom invited to participate in symposia organized by historians of science, and most are loath to publish in such journals as *Isis* or *The British Journal for the History of Science* for fear of negative reviews.

Future Prospects

I do not see the liaison between chemical historians and historians of science improving any time in the near future, but rather suspect that it will further deteriorate. This prediction is based on current trends in the history of science community.

The first of these is the fact that very few current historians of science are willing to be explicitly identified as being primarily historians of chemistry. When I was a graduate student at the University of Wisconsin there were three faculty within the history of science department that specialized in history of chemistry: Aaron Ihde, Robert Siegfried, and Erwin Hiebert. By 1990 there were none. Current historians prefer to be generalist rather than historians of a particular branch of science (with the possible exception of medicine). Though in recent decades historians have produced any number of significant books on the history of chemistry, these are almost all based on their doctoral theses, and after their publication we hear no more of the authors as they are off in pursuit of some other interest unrelated to chemistry. This is the primary reason that very few explicit courses in the history of chemistry are offered by history of science departments.

The second reason has to do with the difference in how chemists versus historians are trained. A doctoral candidate in history is required to present and defend a truly novel thesis. This usually requires that he dismiss everyone who has previously written on the subject in question as incompetents who have completely misunderstood the history they are writing about and claim that only the candidate's proposed interpretation is the correct one. Lavoisier and the first chemical revolution have been particularly susceptible to this reinterpretation craze, often with highly distorted results.

Connected with this is the increasing tendency, depending on the latest historical craze, of employing informal terminology and strange viewpoints when titling books and papers. Thus the book on the Dartmouth instrument collection in reference 14 does not have a straightforward title, such as *The Dartmouth Collection of Historic Scientific Instruments,* but rather the uninformative, if not misleading, title of *Study, Measure, Experiment: Stories of Scientific Instruments at Dartmouth,* almost suggesting that it is a children's book dealing with the scientific method. If I am to judge from the titles of many of the books sent to *Isis* for review, this is a very mild example of this trend.

Conclusion

In summary, history of chemistry has a future, but that future will not differ much from its past.

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REMOTE INTERVIEWING AND THE HISTORY OF CHEMISTRY

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Abstract

Several distance interviewing techniques used by the author since the early 1980s are presented along with examples that illustrate various issues dealing with some social aspects of history: the roles of culture, credit, and priority in chemistry. Remote interviewing, especially by email and videoconferencing, are shown to be highly effective and perhaps even the optimum methods for interviewing subjects for research in the history of modern chemistry.

Preface

Every source of data is useful and potentially critical in the study of history of chemistry (HoC). All historians would, or should, agree that if possible, interviewing actors involved in historical events is of critical importance in the study of the history of those events. Indeed, interviewing even witnesses to historical events in science—others in the relevant peer communities—can provide insights and clues that go beyond what is available from the relevant literature. This essay is about distance interviewing methods I have used over the past 40 years, focusing on transformations of methodologies that have occurred over that time in research in the HoC.

Introduction

There is a sweet spot in the study of history of science, where the actors and members of their peer group—witnesses, even supporting actors to extend the metaphor—are still alive and are sufficiently chronologically distant from the events to feel free, even enlivened and empowered to discuss their experiences. They can even do so with fresh eyes, frequently with sharp memories, and often though not always with receded if not mellowed emotions. With age can come a sense that sharing information from the past is socially and ethically acceptable and even a responsible activity of a scientist. Furthermore, current scientists are especially interested in the history of their fields, especially when they have personal connections with the events, the science and the actors themselves.

The visible portion of the scientific enterprise consists primarily in the published and unpublished documents as well as the inventions and discoveries that have been tangibly memorialized. Enormous as the scientific literature is, what we see is just the tip of the iceberg of the enterprise that is science. A vast percentage of the activities of science is out of sight, and with the death of the actors, becomes lost to time.

For my research over the past 40 years, I have conducted several forms of "remote interviewing" which includes interviewing by letters, fax, and now, especially by email. Rarely have I used on-line video interviews; indeed, in my research and in this paper, I address *only* remote written interviewing. I shall not discuss oral histories, as I have never conducted any—though I have used many in my research to great advantage. Also in this paper, I shall provide examples of remote interviewing over the course of my career that involve the social-cultural context of science. Examples were chosen to illustrate the effect of culture on priority claims and credit, themes that are central to the motivation of scientists and thus to the progress of science (1, 2).

Distance Interviewing by Mail

My first example deals with private agreements among scientists to divvy up research areas, unilaterally contravened representations, multiple simultaneous discoveries, and asymmetric relationships.

In 1980, I was invited to write a chapter on an aspect of reaction kinetics for a book series entitled *Advances in Chemistry.* I decided to include a brief history of the subject in my chapter. I wrote letters to all the leaders in the field, posing questions and requesting photographs. Every single chemist responded including one Nobel laureate, Derek H. R. Barton. Excerpts from Ernest L. Eliel's letters are particularly informative.

Eliel (1921-2008) (Figure 1) was to become a member of the National Academy of Sciences (NAS), president of the American Chemical Society (ACS), and recipient of the Priestley Medal, the highest award in chemistry in the United States. In response to my letter inquiring how he came to discover an important principle in chemistry, Eliel responded on September 22, 1980, by letter. He wrote, in part (3),

> The first ideas of conformational analysis in mobile systems surfaced in a paper I wrote in 1952 … In the summer of 1953 Saul Winstein visited Notre Dame for an extended period as Reilly lecturer and I asked him about the extent of his own interest in doing quantitative work in conformational analysis. At that time Winstein indicated that he was only interested in assessing conformational effects on solvolysis … In 1954 I did a great deal of thinking about [this subject and have several witnesses to that fact]. The clarification came to me in the late fall of 1954 … I was rather taken aback when in January 1955 I received a preprint of the famous Winstein/Holness paper. Winstein obviously had changed his mind about strictly working on solvolysis … .

In the early 1950s, Eliel was a recent refugee from Nazi Germany. He had spent most of the war years in Cuba, received his Ph.D. in chemistry in 1948 (University of Illinois) and in the fall of 1948, Eliel became an instructor at Notre Dame University. Thus, when Eliel was misled by Winstein's misrepresentation, he (Eliel) was low on the academic totem pole. On the other hand, Winstein was entering the height of his powers (he was elected to the NAS in 1955). Eliel held his tongue and did not confront Winstein.

Figure 1. *Ernest Eliel, reportedly about to mail the manuscript for his famous book* Stereochemistry of Carbon Compounds *(4), Notre Dame post office, ca. 1959. Photograph courtesy E. L. Eliel.*

In his 1965 book on *Conformational Analysis,* Eliel very mildly asserted his priority without engaging Winstein's ethics. Eliel documented his priority over Winstein in a footnote (5),

> Following earlier speculations on the conformational behavior of mobile systems (E. L. Eliel, *Experientia,* **9**, 91 (1953)), E. L. E., in the fall of 1954, developed the quantitative expression … and communicated some of the results to Professors W. G. Dauben and D. Y. Curtin (private communications, dated December 20 and December 22, 1954). In January 1955, Professor S. Winstein kindly sent to E. L. Eliel the manuscript [containing the breakthrough Winstein-Holness equation] … Thus [Eliel's equation and Winstein's equation] were developed independently in the two laboratories … .

From my experience with Eliel and also from seeing several other examples of similar joint-yet independent research strategy planning in letters by such eminent scientists as John D. Roberts, Roger Adams, and William von E. Doering (6), I conclude that:

- Researchers privately, even covertly, divide research programs among themselves with the rationalization that they are reducing waste in granting agency funds, minimizing duplicative research, and protecting students' educational trajectories.
- These agreements are not always maintained. Practical (promotion, funding) and emotional (being scooped) consequences can lead to per-

manent damage in relationships. An excellent example of an agreement not maintained was one by Geoffrey Wilkinson and Ernest Otto Fisher in the spring of 1954. While they agreed on some division of the periodic table in the study of the sandwich compounds, e.g., ferrocene-type compounds, neither group abided by that agreement (7).

- Sometimes discussions regarding overlapping research interests lead to collaborations rather than competition. As Albert Eschenmoser described the decision to form the Woodward-Eschenmoser collaboration on the total synthesis of vitamin B_{12}, “We decided it was better to collaborate than to compete” (8).
- Asymmetrical relationships can minimize outward conflicts though emotional turmoil can be permanent.
- Strong emotions and previously hidden conflicts can be revealed even during remote interviews.

By 1980 when Eliel wrote that revealing letter to me, he and I had built a close professional relationship. Eliel knew of my chemical research, and we had corresponded frequently. On a trip to Richmond where I live, Eliel had visited me in my home. Faith in one’s interviewer matters. There are many ways to break trust and only one way—eternal vigilance—to maintain trust. I’ve discovered that most individuals want to share, and they are happy to reminisce. They are pleased that someone is interested in them and their lives. It helps if they also recognize your credentials and your knowledge.

Interviewees sometimes say to me, “What I am now going to say is confidential.” I generally agree immediately. Rarely do I ask that interviewees *not* divulge anything that is confidential; sometimes interviewees withdraw that condition, because human beings want to be heard, understood, and valued. Usually, I share advanced drafts of my writings to interviewees for their review, not just as a courtesy, especially if I perceive there are sensitivities involved. And I very much appreciate that opportunity when the roles are reversed.

Only once in my 40 years of interviewing was I told three hours into a major in-person (telephone) interview, “Of course, everything I’ve just told you is confidential.” I responded, “Nothing you’ve just told me is confidential. Confidentiality must be agreed upon *before* an interview, *not after.*” The interviewee agreed immediately, and we continued the interview for another 30 minutes. He wanted to be heard. But I subsequently provided him two advanced drafts of my manuscript, and I revised my draft based on his corrections and clarifications. That being said, my relationship with that chemist was permanently damaged. I could have, likely should have, responded more softly and reassuringly, not spontaneously like an attorney.

A colleague has asked, “What do you do about highly embarrassing or even tragic life events that you’ve learned about a dead person?” A life principle of one of my chemistry heroes Vladimir Prelog was, “*De mortuis nil nisi bonum*.” (“Of the dead, say nothing but good.”) Do we reveal tales of marital infidelity, for example? One must think deeply and question mightily: Was this information ill-gotten? Is it substantiated? Will a true and complete history of science be forsaken with its absence? And does one have—or need to have—permission from a family member to reveal such information? I am just now dealing with one truly tragic life experience and the privacy of the subject and their family.

Communication by letters is slow, even slower today than 40 years ago. But in those days, I found distance interviewing by mail to be effective and inexpensive, and it provided a wonderful collection of autographs of eminent chemists!

Beginning in 1983, I conceived of, organized, contracted with a publisher (the ACS), and edited a series of 20 autobiographies of eminent organic chemists (9-11). Living in seven countries, the authors represented all the major sub-disciplines of organic chemistry. Five were Nobel Prize laureates, and all of them were the elite of their fields. The project entitled *Profiles, Pathways and Dreams* had several goals. One was to illustrate how individual research programs evolved over many decades; the average age of the authors was well over 70. And when taken together, the books revealed how organic chemistry had evolved from the 1940s into the early 1990s. There was great diversity among the authors, in terms of subdiscipline and personality. But not in terms of race and gender, unfortunately. All the authors were Caucasian except two who were Japanese, Tetsuo Nozoe and Koji Nakanishi. All were men. As one of this paper’s reviewers wrote,

> I do not think that the author has excluded on purpose minority/female organic chemists. It was the way the field of organic chemistry was at that time, populated mostly with white male scientists.

I appreciate that understanding. That was the way it was. Today, the series would be far more inclusive and diverse.

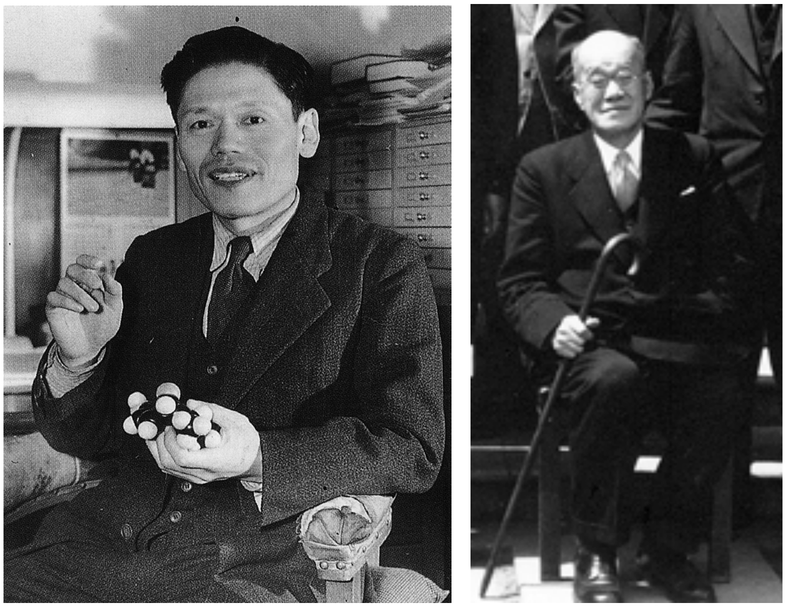


Figure 2. *(left) Tetsuo Nozoe, 1952. (right) Riko Majima, 1958. Photographs courtesy T. Nozoe.*

Without my request or anticipation, many authors sent me their manuscripts chapter-by-chapter (by mail!) for my review. I rapidly became immersed and excited in these life stories. I constantly asked for more from the authors. I wrote questions in green ink within the white spaces of the typewritten manuscripts. When my commentary was long, I used an early word processor and inserted individual pages within their draft, then sent a collated package back to them. When a revised draft reached me, I would compare it with my annotated version. It was like magic. I was surprised by many discoveries. Many years ago, I concluded:

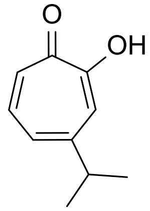
- An editor is automatically given an aura of respect and influence. An interviewer often has the same standing.
- Reasonable questions will most always be answered.
- Results are proportional to the interviewer's preparation and sometimes persistence.
- An interviewer's job is being the servant of the author.

Distance Interviewing by Fax

Distance interviewing is generally necessary for individuals who live in countries quite distant from the interviewee. But interviewing such individuals also comes with other challenges: language and cultural considerations. Fortunately, English seems to have successfully become the *lingua franca* (12-14). But differences in cultural norms can affect both science and scientists.

In the West, little is known of the history of Asian chemistry. For example, the identities and life stories of the foundational Japanese chemists are relatively unknown outside of Japan. Many Japanese historians of chemistry often write in Japanese (15-17). Even some of the great Japanese chemists, e.g., Kenichi Fukui, wrote their autobiographies in Japanese (18), and unfortunately, it is only in their first language that those autobiographies were published and accessible only to readers of East Asian languages. Was Fukui's autobiography, for example, considered by the publisher not to have a market outside of Japan? Erich Hückel's autobiography (19) remains solely in German. But Richard Willstätter's autobiography (20) was translated from German to English. All the autobiographies in the *Profiles, Pathways and Dreams* series were published in English (though Vladimir Prelog's autobiography (21) was initially written in German by Prelog and translated into English by David Ginsburg and O. T. Benfey), an example of the application of a *lingua franca* and perhaps also the fact that the publisher was the American Chemical Society.

As mentioned above, one of the *Profiles* authors was Nozoe (1902-1996) (Figure 2), the doyen of late 20th century Japanese chemistry. Nozoe was first to discover the structure of a non-benzenoid aromaticity (hinokitiol), though his achievement was published in Japanese in the early 1940s and so was recognized in Europe and America only *after* Michael Dewar in England and Holgar Erdtman in Sweden had made their simultaneous independent discoveries in the late 1940s (22) Nozoe's professor in the early 1920s was Riko Majima (Figure 2) (23, 24). Majima (1874-1962) was the seminal Japanese chemist from whom the first generation of major Japanese organic chemists was produced.



Hinokitiol

I asked Nozoe to provide a listing of Majima's most successful and consequential students (first generation Majima descendants) and then a listing of the most important students of those professors (second generation Majima descendants). This is equivalent to family genealogical trees that trace one's family's ancestors. Within a short time, I received a fax containing Nozoe's derivation of Majima's family tree. A day or two later, I received a fax from Nozoe, that he was deleting the Majima family tree from his autobiography.

Nozoe had shared the family tree with some of his colleagues and was very strongly advised *not* to publish it. As Nozoe could not list every student of Majima's, by including some names and excluding others, Nozoe would be making public judgements about academic caliber. This would be a significant taboo within the Japanese culture which values harmony, group (which equals "family") loyalty, and the maintenance of good human relations (25-27).

What was I to do? Nozoe, then in his late 80s, was the last living person who could authoritatively document the record of early 20th century Japanese organic chemistry. It was now or never. I explained this conundrum to Nozoe. Multiple faxes went back and forth between us. Which would Nozoe choose: history of chemistry or the maintenance of cultural norms? Ultimately a very brave Nozoe chose HoC.

- For Nozoe to include the Majima family tree required Nozoe to face squarely his place in the HoC as well as his obligations to the culture in which he lived.
- With the development of mutual trust, the bond between interviewer and interviewee can rapidly become intimate. Responsibilities emerge for the editor to protect the author. Indeed, an interviewer must commit to an Editor's Hippocratic-like Oath: to do no harm, to protect the interviewee (and the author).
- My often almost daily conversations with Nozoe via fax built this trust and negotiated complicated issues smoothly and diplomatically. Thirty years after the publication of Nozoe's autobiography and 25 years after his death, we have this important documentation of the leaders of early 20th century Japanese organic chemistry.

For 40 years, from 1953 to 1992, Nozoe collected autographs and other writings during his worldwide travels. Many of these were published in his autobiography (22). You can watch a short video produced by Carman Drahl and *Chemical & Engineering News* which includes short interviews of Roald Hoffmann and Carl Djerassi and me (!) discussing the Nozoe autograph books:

https://www.youtube.com/watch?v=pqswFQrUdw8.

Between 2012 and 2015, *The Chemical Record*, a Wiley-VCH journal published for the Chemical Society of Japan, published nearly 1200 pages of Nozoe's travelling autograph books in 15 consecutive issues of the journal (28). This idea was imagined by Eva Wille, a Wiley-VCH senior executive, to whom I actually "pitched" the idea of publishing all Nozoe's autograph books in a single volume. A strong relationship between authors, editors and publishers is critical, not just to "sell a book idea" but to bring it to its maximum fruition. The publication of the Nozoe autograph books was due to my relationship with Wille—and that it was a grand idea to do so!

Distance Interviewing by e-Mail

Distance interviewing has morphed considerably over the past 20 years. Letters and fax have been replaced by email. I shall give several examples of the use of email interviewing to determine the priority of achievements dealing with the development of the Woodward-Hoffmann rules published in 1965 by R. B. Woodward and Hoffmann (29-33). In 1981, Hoffmann received the Nobel Prize in Chemistry for this achievement. Had Woodward not died in 1979, he would have received his second Nobel Prize. In 1965 Woodward received a Nobel Prize in Chemistry for his total syntheses of complex natural products.

First, I shall discuss the Charles H. DePuy (Figure 3) story. In 2016, Veronica Bierbaum and Robert Damrauer, two professors at the University of Colorado, published a biographical memoir for the NAS of their former University of Colorado colleague Charles DePuy (1927-2013). Within their memoir, Bierbaum and Damrauer wrote (34),

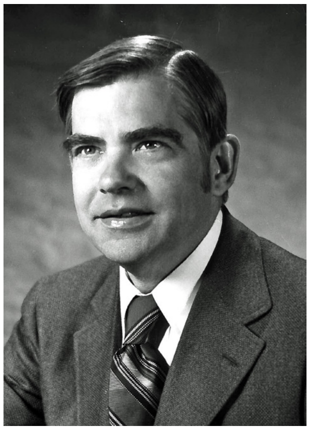


Figure 3. *Charles DePuy, ca. 1965. Photograph courtesy C. DePuy.*

> [DePuy] did comment to friends that such ideas [the stereochemistry of ring-opening in cyclopropanol

> solvolyses] had been raised with Roald Hoffmann at a meeting in October 1964, but they had not been attributed to Chuck in Woodward-Hoffmann papers until sometime later.

The implication is that Woodward and Hoffmann slighted DePuy. From my email interviews with Hoffmann, I knew the story was more complicated than what appeared in the NAS memoir. In fact, while Woodward and Hoffmann did fail to credit DePuy in their first 1965 paper (29), they cited DePuy fully in their reviews of the topic in 1968 (35) and in 1969 (36). In an email interview with me (37), Hoffmann acknowledged that he and Woodward

> did not credit him properly. He complained, rightfully. We made up for it in [subsequent papers].

Recently I emailed Bierbaum and Damrauer. I asked them several questions.

> JIS [Seeman]: By your inclusion of this matter in your memoir, are you implying that Chuck held any, even the smallest, degree of dissatisfaction with Woodward and/or Hoffmann regarding attribution?
>
> B&D [Bierbaum and Damrauer]: Yes (38).
>
> JIS: If yes, then was this your attempt to further set the record straight?
>
> B&D: Yes (38).

Fortunately, I had interviewed DePuy on this credit matter. On July 17, 2011, DePuy wrote in an email (39),

> To be perfectly honest, I did not notice until many years later that the cyclopropyl case was covered in the initial [1965] Woodward-Hoffmann communication. I guess I thought I knew what the communication was about and did not read down to the last line. I did notice their acknowledgement in their [1969] book, which seemed strange but welcome. Still, I do not believe that anyone behaved at all unethically and my hearing about the W-H rules at the [October 1964] Natick meeting gave me wonderful ideas for some very interesting chemistry.

Thus, Bierbaum and Damrauer's claim on behalf of DePuy against Woodward and Hoffmann in the NAS memoir is inconsistent with DePuy's position. I felt I had an obligation to help set the record straight. I wrote to them both. In a prompt email response, Bierbaum and Damrauer revised their understanding, writing to me (38),

> We were not directly involved in the W-H issues and so don't have additional information. It's good that you were able to interact directly with Chuck before his passing; your reporting of these communications in your *Journal of Organic Chemistry* paper is the best reflection of Chuck's thoughts on the matter.

But their internet-available memoir stands unchanged (34) though this paper helps to set the record straight.

Next I shall tell a story involving the photochemist Howard E. Zimmerman (1926-2012) (Figure 4). Zimmerman, a former student of Woodward's, was a professor of chemistry at the University of Wisconsin for many decades. In his 2014 biographical memoir of Zimmerman also for the NAS, Richard S. Givens, a former graduate student of Zimmerman's and professor at the University of Kansas, wrote that in 1961 (40)

> Howard [Zimmerman] was among the first to employ orbital *correlation diagrams* in assessing "allowed" and "forbidden" pathways for reaction processes controlled by orbital symmetry … [emphasis added]

Figure 4. *Howard E. Zimmerman, Madison, WI, ca. 1980. In this photograph, Zimmerman is shown before a map of the world in which he placed brightly colored push pins to mark the location of his former students who held academic positions.*

In their second 1965 communication (30), Woodward and Hoffmann used *correlation diagrams* as the theoretical basis for their proposed mechanism for cycloadditions but did not cite Zimmerman. In 1961, Zimmerman and Arnold Zwieg derived a "molecular orbital reaction diagram" without symmetry assignments—a required component of correlation diagrams—and used LCAO-MO calculations as supporting evidence for the mechanism of several carbanion rearrangements (41). In his June 5, 2020, email responding to this author's email of June 4, 2020, about correlation diagrams, Givens corrected himself (42),

> In answer to your question, the paper you cited for Zimmerman and Zwieg does not involve *correlation diagrams* but rather, questions of orbital overlap and electron population to determine … . [emphasis added]

Thus, Givens agreed with my analysis: Zimmerman's 1961 paper with Zweig (41) did not include correlation diagrams.

I actually had interviewed Zimmerman quite extensively shortly before his death. Among many responses to me, in an August 7, 2011, email, Zimmerman described his own contributions to the field (43):

> It was tragic for me that I had not seen the generality of Arnie Zweig's *correlation diagram* other than in the paper [*sic*] we did make clear that occupied bonding MO's going antibonding impede the reactions … I have no claim on early discovery… . My 1966 Möbius-Hückel article is where my interest begins. [emphasis added]

Zimmerman thus acknowledged that he had no claim, but he mischaracterized his 1961 publication. Zimmerman also believed he had presented a correlation diagram, and indeed, Zimmerman and Zweig were tantalizing close to have done so. But they did not.

I conclude,

- As scientists well know, science is complex, and so is writing about science. Often only subject-matter experts can examine the historical record in order to characterize correctly the science.
- Errors in attribution are easily made and hardly ever corrected. These are typically neither intentional nor deceitful. Nonetheless, attribution errors often remain permanently in the record, as the last statement of priority.
- Errors in remembering and characterizing one's work are often made. These are not always intentional. Robert K. Merton, the great sociologist of science and one of my heroes, used the term cryptomnesia (2, 44). According to Wikipedia, "Cryptomnesia occurs when a forgotten memory returns without its being recognized as such by the subject."
- Authors of biographical memoirs are often "academically-related" to the examinee, as former students or colleagues are most apt to write such treatises (and are most apt to be invited to do so). Various biases are possible if not likely, e.g., favoritism bias and conflict of interest bias. In these instances, attributions of credit must be made very carefully by the authors and considered very carefully by readers, if they are even aware of the familial relationship.
- As Merton discussed in detail, credit is a primary motive among scientists and an important issue for the history of science (2, 45). Great care must be done by biographers and others who attribute credit in their writings.
- Emailing is a rapid and highly interactive mode of distance interviewing.

Additional Observations and Conclusions

I have discovered that some individuals prefer telephone interviews to questions by email. There is little hope to convince a determined telephone-interviewee to do otherwise. Recording such a telephone interview is optimum. Otherwise, inaccuracies can enter the historical record. I much prefer distance interviewing by email. Interviewing by email is not unlike traditional letter correspondence or even oral histories regarding the interviewees' freedom to craft their narratives.

A reviewer has asked,

> How do we judge the validity of eye-witness reports? How do historians treat the biases of the interviewer and the interviewee?

These topics have generated a large and rich scholarship, for they are a very lively concern in the field of history of modern science. Trouble brews when individuals are inconsistent in their own responses or when the stories of different actors do not coincide. This concern is valid for all forms of interviewing. I have faced such instances several times. The following techniques have proven useful in my research: I attempt inquiry via different substantive trajectories; I seek testimony from multiple actors; I relentlessly examine testimony for consistency in responses over time for the same event; and I refer to published and unpublished documentation. Sometimes we simply must accept and document inconsistencies in the record. People are not always consistent in their behaviors.

Life is rich with vagueness (46-48). At such times, distance interviewing by email is especially useful; it is easy to inquire several times, over several days, to multiple individuals. Even faced with Rashomon's tribulations (49, 50), one never, ever alters an interviewee's narrative to fit one's interpretation of events or to be consistent with the memories of others or even to agree with relevant contemporaneous documentation.

There is another aspect of email interviews that ought to be highlighted: Interviews by email easily allow one to pursue newly opened areas of interest and clarify any possible ambiguities. All one needs to do is send another email loaded with the appropriate questions. Repeatedly, I find folks all over the world who immediately, happily, and rather spontaneously respond to emails. In my major current project on the history of the development of the Woodward-Hoffmann rules (51), which includes E. J. Corey's claim of plagiarism against Woodward (52, 53), I have hundreds of emails from Hoffmann and tens of emails from others who have been involved in this multidimensional story. The brightest times of my day are when I see a response in my inbox.

Looking Toward the Future

I do believe that modern distance interviewing—by email—is not just easier and faster than previous methods. It also provides more and more rapid opportunities with individuals who share rich historical data and very personal perspectives. I also believe that the future will provide possibilities in distance interviewing far beyond our anticipations. Even today, one can imagine video interview segments being included in journal articles that are accessed on-line– just as I have included a *url* link to a short video about the Nozoe autograph books herein. With character recognition, rapid on-line translations, and artificial intelligence-facilitated capabilities not yet even imagined, the ability to bring HoC to the world's communities at levels from kindergarten to research level is unlimited. Distance interviewing and recording on-line video interviews provide additional, powerful incentives for the study of the history of modern chemistry—a topic mostly avoided by professional historians (11).

Hoffmann has characterized scientists as "scrabblers" (54). I claim that all researchers, including historians of chemistry, are scrabblers. Scrabblers seek more and better information for their research using whatever tools and resources are at their disposal. Some researchers are more enterprising if not enthusiastically ambitious, in their pursuit of information. Others are less so. Such is the way of research and of interviewing.

Coda

An unstated assumption in this paper is that the history of modern chemistry is a legitimate historical endeavor. In another article in this special issue of the *Bulletin* (55)*,* Peter Morris and I have briefly discussed the need for an increased study in the history of modern chemistry—a topic that Morris has spoken of previously (11). I have been told informally by several historians that science must be at least 25 years old to be considered appropriate for a study of the history of chemistry. In another article in this special issue, Carmen Giunta argues otherwise, and quite persuasively (56). It is quite telling that the philosopher of science Thomas S. Kuhn wrote (57):

> [The history of] science should be learned from the textbooks and journals of the period he studies.

Besides using the term "he" to represent historians of chemistry, an affront to today's sensibilities and realities, Kuhn, in his quote, did not consider interviewing scientists who were participants or active observers of the historical events. This is, of course, the entire subject of my present paper and many of my own contributions to the history of chemistry.

I owe a debt to Derek H. R. Barton (1969 Nobel Prize in chemistry); I follow quite willingly Barton's precedent (58) for my use of codas in my own writing.

Coda to a Coda

Since the submission of this paper, I have begun conducting interviews using Zoom and Skype, during which I type my subjects' responses to my questions as if I were a court reporter. Video interviews have been accomplished quite effectively with Roald Hoffmann and Sason Shaik. The interactive nature of such interviews provides for enormous flexibility in topic and for intense focus on issues that arise during the sessions. Hoffmann and I have each drawn graphics and showed these and other documents to each other using the video camera or by concurrent emailing of attachments. These video interviews have lasted from one to two hours and must now be considered another and very effective form of distant interviewing.

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About the Author

Jeffrey I. Seeman received his B.S. in chemistry from Stevens Institute of Technology, Hoboken, New Jersey, and his Ph.D. in chemistry from the University of California, Berkeley. He was a research chemist for over 30 years in industry and a fulltime consultant in the field of chemistry for another 10 years. In 1983, Seeman published his first paper in the history of chemistry. His first career highlight in HoC was the creation and editing of a 20-volume set of autobiographies of eminent organic chemists entitled *Profiles, Pathways and Dreams* which was published by the ACS from 1990 to 1997. In 2007, Seeman accepted a courtesy appointment in the Department of Chemistry at the University of Richmond in his hometown in Virginia. As his work in chemical research decreased in magnitude in the early 2000s, his research in the HoC correspondingly increased to the extent that today it consumes most of his professional time.

IS THERE ROOM FOR THE PRESENT IN THE HISTORY OF SCIENCE?

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Abstract

With due appreciation for insights of historians, sociologists, and philosophers of science about the contingency of history in the making, the susceptibility of grand narratives to propagandistic purposes of the narrators, and of the tentativeness of scientific knowledge, I propose that an eye on the present, prudently and consciously applied, can sometimes be illuminating in history of science. For at least one class of readers and writers in history of chemistry, namely chemists, the question of "how did we get here?" is a natural intellectual one. The question need not—ought not—imply that "here" is an inevitable or a final destination. Why narratives that refer to the present appeal to chemists is discussed, as are some of the pitfalls to which such narratives are prone. Historians of chemistry are invited to reconsider some aspects of their professional strictures against keeping an eye on the present.

Introduction

The portrayal of figures from the past can lead to strong responses in the present, as was apparent when statues became foci of protests in reaction to the killing of George Floyd by Minneapolis police officers in 2020. In the United States, monuments to people who had owned slaves or fought for the Confederacy during the Civil War were particularly contested, as were statues of Christopher Columbus. Debates over the memorials were often heated: those who urged removal argued that the monuments glorified white supremacy, while those who defended the statues asserted that removal was tantamount to erasing history.

What does this have to do with history of science? For one thing, scientific figures are not immune from this public reassessment, as Sebastian Kaupp-Roberts illustrates in a short piece about the nineteenth-century American surgeon J. Marion Sims (1). Sims invented useful gynecological procedures and instruments, some of them developed while operating without anesthesia on enslaved women—after anesthesia had been successfully demonstrated. City authorities in New York ordered the removal of a statue of Sims from Central Park in 2018.

For another thing—more relevant to the essay that follows—the monument controversies prompted widespread discussion in the popular press and social media about judging the past by standards of the present. Again, science was not exempt, as exemplified by an opinion piece in the *Financial Times* headlined "Scientific History Should Not be Set in Stone" (2) and a short responding letter "Don't Judge Historical Figures by Modern Values" (3).

I wish to pursue the influence of present-day issues, knowledge, and values on the depiction and understanding of the past in science. Having begun in arenas visible to the wide world, I turn my attention to the scholarly world—without losing sight, I hope, of communication to a wider public (4). In short, I offer some opinions about a recurrent topic in historiography, and particularly in historiography of science under the headings of presentism or whiggism. I propose that some aspects of whiggism can be present in scholarship of high quality, and I suggest why scientists have some affinity for whig history for good and for ill. I would be pleased if some professional historians of chemistry who read this article consider relaxing the rejection of presentism ingrained in the profession and if some fellow chemist-historians recognize some of the deleterious aspects that can accompany presentism.

What is Whig History and What is Wrong with It?

Whiggishness or whiggism is a term of opprobrium in the field of history, including (or perhaps especially) in history of science. The term whiggism appears first in Herbert Butterfield's influential book *The Whig Interpretation of History*, originally published in 1931 (5). Butterfield generalized the term from a reference to British political history written by members of the Whig party or scholars sympathetic to their aims. Such histories were simple morality tales of progress, culminating in the Whigs and their policies. By extension, whig history is any overly simplified historical narrative, presenting actors in the past either as promoters of the glorious present or obscurantist opponents of it.

Butterfield points to a preoccupation with present concerns as the root of this sort of bad history (pp 31-32):

> The study of the past with one eye, so to speak, upon the present is the source of all sins and sophistries in history, starting with the simplest of them, the anachronism.

The problems begin even with the choice of historical question to investigate. A real historian seeks to understand the past in its own terms (p 17):

> Instead of being moved to indignation by something in the past which at first seems alien and perhaps even wicked to our own day, instead of leaving it in the outer darkness, he makes the effort to bring this thing into the context where it is natural, and he elucidates the matter by showing its relation to other things which we do understand.

Butterfield goes on to contrast the true historian with two others, the first of whom, perhaps, is no historian at all, while the second is a whig historian (pp 17-18):

> Whereas the man who keeps his eye on the present tends to ask some such question as, How did religious liberty arise? while the whig historian by a subtle organization of his sympathies tends to read it as the question, To whom must we be grateful for our religious liberty?

For Butterfield, the remedy to whiggish approaches to history is thorough and detailed historical research that enters into the concerns and categories of the past, describing it in all its complexity and in its own terms. Abridgement is suspect, in his eyes, although he admits that it is necessary: it must be done, but in such a way that does not change the meaning of the narrative. The whig historian, by contrast, has an easy principle of selection that cuts through the complexity, namely to concentrate on the people and institutions whose ideas most closely resemble our own.

Objections to Butterfield's Strictures

Butterfield was certainly correct to criticize writing about history in a way that portrays figures of the past as having concerns and motivations that refer to the present, i.e., as promoters or opponents of what became the present. Such narratives distort how and why past events unfolded, and they lend themselves to simplistic teleological tales of heroes and villains. But is it really necessary, if one is to write good history, to leave the present out completely? As Nick Jardine puts it (6):

> With Butterfield we surely should reject the hagiographical elevation of past "friends of progress," the structuring of historical narratives as fated convergences onto present beliefs and institutions, and the uncritical projection of present values onto the past. But there is no need to throw out the baby with the bath water.

There are two particular ways that I would suggest the present can be brought to bear in history of science in ways that would not diminish, and could enhance, its scholarly value.

1. In selecting historical questions based on interests in the present, including tracing a development from its discovery or proposal through to its present status.

2. In using present scientific knowledge judiciously to interpret past experiments and observations.

It seems to me that the present can be drawn into history of science in these two ways regardless of any philosophical commitment for or against the notion of scientific progress. I then discuss why a philosophical belief in scientific progress (to be defined below), common among scientists, makes whiggish history of science appear natural, for good and for ill.

Selecting Questions for Investigation

My first reaction to reading Butterfield's opinions about questions asked by those who have their eye on the present was that those are just the sort of questions scientists curious about the past of their field would ask.

That reaction was hardly original. Rupert Hall, writing about whiggism in 1983, observes, "The most obvious of all historical questions is: 'How did we arrive at the condition we are now in?'" Academic historians might be trained to avoid putting such questions, but, Hall notes, "The question is put, and the questioner will find an answer somewhere; if academic historians are silent he or she will seek an answer in other ways" (7). Hall laments the lost opportunity to communicate to those outside the field of history who pose such questions. After all, he suggests, who better to give reliable answers, including relevant contingencies and uncertainties, than historians?

Ernst Mayr describes a more refined version of the question of how the current situation came to be. Mayr (1904-2005) was a distinguished evolutionary biologist (elected to US National Academy of Sciences) who also wrote about the history and philosophy of his subject. He defines developmental history of science as "the study of those aspects of the past that help our understanding of the science of the present" (8), and he asserts that questions of this sort are what interest practicing scientists in the history of their fields. He distinguishes developmental history from descriptive history, the latter narrating how events unfolded in time. Good developmental histories, he asserts, do not ignore "failed" ideas, although they do not spend as much time on them as on theories whose traces are still visible in those of the present. Describing the development of a scientific discipline to the present need not—should not—assume that present theories are final.

Mayr argues that developmental history of science is not whiggish and that it is legitimate. If we take Butterfield's definition ("eye on the present"), developmental history of science ***is*** whiggish, but I agree with Mayr that it is legitimate. As scholarship, it ought to be judged in terms of what it sets out to accomplish, namely to trace ideas that shape current theories in a field. It seems to me that Mayr's developmental history is an extension of the "temporal depth" Edward Harrison mentions as "an integral part of scientific research" (9). Certainly scientists' networks of citations to earlier publications can function as source material for investigating the development of ideas in a field.

Naomi Oreskes touches several themes similar to Hall's 30 years later in an essay provocatively titled, "Why I Am a Presentist" (10). To be clear, Oreskes considers herself a motivational presentist only (that is, someone whose historical interests are influenced by the present), not a substantive or methodological presentist. Substantive presentism, she writes, is a belief that the past is substantially like the present; methodological presentism seeks to understand the past by studying similar events in the present or recent past. In her view, historians are right to avoid those two forms of presentism. But as for why historians write history (p 604):

> We believe it is of value to us—living here, today, at this moment and in this place. If we deny this (really rather obvious) fact for fear of being labeled "presentist," we deprive ourselves of the most important argument we have for why we do what we do, why our universities and funding agencies should underwrite it, and why our students should be required to study it.

For Oreskes, topic selection rooted in the present need not be the question of how we got to the present; however, for her, as for Hall, relevance to the present would give historians opportunities to communicate with the wider public or with policymakers or specialists in other fields—opportunities too often forgone.

Using Present Scientific Knowledge to Interpret the Past

Butterfield's exhortation to his fellow historians to "make the past our present" (5, p 16) was made explicit for historians of science by Thomas Kuhn (11):

> Insofar as possible (it is never entirely so, nor could history be written if it were), the historian should set aside the science that he knows. His science should be learned from the textbooks and journals of the period he studies.

Understanding science from within the time it was carried out is certainly important for describing how the activities in question unfolded. I can see how "translating" an operation (a chemical reaction, for example) into modern terms could entail distorting the operation (for example, unconsciously picturing the reaction being carried out with materials as pure or well-characterized as those available from a present-day chemical stockroom). Still, an historian who has immersed herself in the world of a past chymist has the task of interpreting that world to readers in the present. Part of the readers' job is to attempt to enter that unfamiliar past world, but surely the historian is to act as a guide, using readers' knowledge to help them understand that unfamiliar past world.

Arguably, the further removed from our own time, the more danger there is for a reader in the present to misapply current categories to the past. A well-known example is the word scientist, not coined until the 1830s. Using the term to describe an eighteenth-century savant practically invites the reader to clothe the savant in the nineteenth- and twentieth-century professional identity that the term brings to mind (12).

The word chymistry serves to distinguish the early modern activity described under that name from the later practice of chemistry. Lawrence Principe does not shy away from meeting his readers in the present, though, when introducing them to chymistry (13):

> Early modern chymistry embraces many topics that are usually regarded today as separate disciplines—chemistry, medicine, theology, philosophy, literature, and the arts.

He goes on to explain why it would be a mistake to think of chymistry as a "protochemistry," but he notes that twenty-first-century chemistry can be brought to bear in understanding it (13, p 138):

> First, a knowledge of the chemical and physical properties of substances can help the historian grasp the processes and ideas that early authors describe incompletely or allusively. Second, and more vividly, a working knowledge of chemistry enables the researcher to try to replicate—and thereby understand better and more deeply—historical processes and results.

Attempting to reproduce experiments has been used to good effect to clarify more recent episodes in the history of chemistry, such as the validity of the formal synthesis of quinine announced in 1944. That announcement was called into question early in the twenty-first century, and experimental investigations published in 2008 supported the announcement (14). Stephen Brush mentions experimental reconstructions approvingly as one way for scientists to bring their skills and knowledge to historical investigations. Brush's essay argues strongly for a place for scientists in history of science "if they are willing to acquire the skills and background knowledge of the historian of science" (15). That proviso, in his opinion, ought not to deter scientist-historians from investigating presentist topics or employing their scientific expertise in pursuing historical questions.

Hasok Chang adopts a pluralistic attitude toward historiography of science, including whiggish and other presentist perspectives. Indeed, the problem with historiography that has often been criticized as whiggish, he writes, is not present-centeredness but triumphalism, celebrating the winners in past scientific controversies, whether or not the ideas persist in the present (16).

It seems to me that such triumphalism is part of what Butterfield critiqued; after all, Butterfield included "to praise revolutions provided they have been successful" among the transgressions of whig historians (5, p v). Still, Chang's distinction is a useful one, for he illustrates how one can be informatively whiggish about phlogiston as a partial antidote to triumphalist narratives about the Chemical Revolution (16). He points out, for instance, that caloric, which is just as imponderable as phlogiston, was a key part of Lavoisier's explanation of combustion. Long after the phlogiston theory had been discarded, practicing scientists proposed possible reinterpretations for phlogiston as chemical potential energy (William Odling in 1871) or as electrons (G. N. Lewis in 1926). I believe that a historical account of phlogiston that describes Odling's and Lewis's suggestions could add to an appreciation of the phenomena that phlogiston explained in its time—albeit clearly in a way that was not accessible to eighteenth-century phlogiston theorists. Similarly, pointing out which ideas of Lavoisier's were subsequently discarded from explanations of combustion illustrates that today's explanation did not spring fully formed from anyone's mind.

More recently, Chang has further developed his ideas on presentist historiography. On the issue of using only the categories available to historical actors, he writes (17),

> For the purpose of reaching the most informative and meaningful description or explanation, there is actually no guarantee, not even a very high likelihood, that actors' categories provide the best framework for it

—as the latter-day reinterpretations of phlogiston mentioned above suggest. Here Chang recommends that professional historians of science generally avoid whiggism, but not because it necessarily produces bad history. Rather,

> The real problem with whiggish history of science is that it always aligns its value-judgements with the current [scientific] orthodoxy.

Chang also notes that scientists can and will produce whiggish history for themselves, and he sees no need for historians to duplicate their efforts.

Why Are Scientists Attracted to Whig History?

Chang is not alone in associating scientists with whig history of science. In my reading on whiggism in history of science, it appears that professional historians of science and scientists interested in history of science agree that scientists often do or did write history of science described as whiggish. Even two pointed commentaries in *Nature* from the 1980s which, respectively, celebrated and deplored professionalization in history of science, agree (at least partly) on this point. Colin Russell describes scientists' forays into history of science as "juvenile improvement or geriatric propaganda" and says that such heroic tales "are really caricatures" (18). Edward Harrison, while characterizing history of science by historians who knew little or no science as "priggish," nevertheless admits that many scientists make unsubstantiated connections and tend toward whiggish abridgments when they discuss history (9). (Differences between professional historians of chemistry and chemist-historians across several dimensions are discussed amicably and in detail elsewhere in this issue in a paper written collaboratively by one of each (19).) And we have seen the biologist Mayr, while rejecting the whiggish label, defend historical inquiry whose object is to elucidate the development of current theories (8).

Interest in relating past science to current science is natural for practicing scientists, who believe that the science of the present generally provides better explanations of how the natural world works and better means for extending that understanding than did science of the past. Indeed, this amounts to a general belief in scientific progress as I understand the term. Scientists appreciate that currently accepted theories are tentative and subject to revision. Still, present theories are naturally accorded a privileged status compared to past ones that have been discarded or modified. In short, practicing scientists generally believe that scientific theories usually become more refined, more reliable, and more comprehensive over time—albeit not inevitably and not necessarily linearly. More fundamentally, belief in scientific progress is accompanied by a philosophical belief in the existence of a real and objective natural world—even if today's scientists never think about the philosophy of science in those or any other terms.

A clear and unapologetic example of belief in the progress of science can be seen in the writings of Steven Weinberg (1933-2021), a Nobel laureate in physics. In science, he notes (20),

> … there are laws of nature, equally binding on all places and times. It is precisely the story of the growing consciousness of the laws of nature that the whig historian of physics hopes to tell, but the story cannot be told without keeping an eye on our present knowledge of the natural world.

Arthur Silverstein, retired professor of medicine, later observes that whig histories of science written at different times would disagree about who in the past was right and who wrong. Weinberg admits the justice of the observation, since current knowledge is not final knowledge, but adds that (20, 21)

> … since the downfall of the phlogiston theory of fire and the caloric theory of heat in the nineteenth century, there has been no generally accepted theory in the exact sciences that has turned out to be simply wrong.

In my opinion, it is important to quote scientists such as Weinberg who are unsympathetic to the project of understanding theories of the past in their own terms or to the suggestion that science is subject to social forces. For example, Weinberg writes that the notion that a scientific theory ought to be judged on how it handled the problems of its own time is "nonsense." He adds "The point of science is not to answer the questions that happen to be popular in one's time, but to understand the world" (20). Apparently there is no room here to see how external factors such as a world war or the COVID-19 pandemic affect "the point of science." To take Weinberg as a model would be to invite dismissal out of hand by historians, philosophers, and sociologists of science who are interested in challenging scientific assumptions and orthodoxies.

Belief in scientific progress need not, indeed ought not, to lead a writer with an eye on the present to simplistic, heroic or triumphalist narratives. Hall notes that in science, some things are wrong and others right. While other historians can see errors in, say, battles or diplomacy, they do not know the right answer; historians of science do. "The historian cannot avoid the burden of superior [scientific] knowledge [of the present]. … Thus, it seems to me, the Whiggish idea of progress has inevitably to be built into the history of science" (7, p 57).

Recommendations that history of science ought to be "divorced from the idea of progress" (7) were made not long after the professionalization of the discipline. But the notion that a belief in scientific progress was intellectually respectable or defensible has also appeared from time to time in history of science journals. Two decades after Hall (7), Nick Jardine opines that the injunction against historical investigation of scientific progress is excessive (6). Still later, the philosopher David Alvargonzález proposes philosophical criteria for assessing the presence or absence of progress in science and technology. While recognizing that many historians and philosophers of science hold that one cannot speak of such progress, he concludes that "recognizing some scientific progress in a sequence of sufficiently large and distant events can only be unanimous" (22).

It is easy to see how a belief in progress, even a progress that is non-linear and contingent, coupled with a consciousness that the present is not the final stage, can lead a scholar to devalue discarded past theories. To take the classic example in chemistry, it is easy to treat the phlogiston theory as an obstacle to understanding combustion rather than to appreciate it as an explanatory framework in its own right. A more recent example might be to regard Linus Pauling's advocacy of the valence bond approach in quantum chemistry as a barrier to more widespread adoption of molecular orbital theory.

It is also easy to see how scientists interested in the past of their discipline but not formally trained in history (among whom I count myself), can fall into the undesirable aspects of whig history. As noted, progressivist narratives come naturally, and can easily turn triumphalist or simplistic if the progressivist assumption is unconscious. It is easy, without critical practice, to make connections between older and newer ideas on the basis of insufficient resemblance, unrecognized divergences in the meaning of terms, or unawareness of differences in purpose between older and more recent actors. With consciousness and practice, these tendencies can be overcome.

Conclusion

I believe that both chemist-historians and historians of chemistry can produce interesting, insightful, and scholarly studies of chemistry and related practices of the past. Such accounts must avoid oversimplification, teleology, and triumphalism, as Butterfield enjoined. But the present need not be barred from such accounts. Chemist-historians ought to be aware of assumptions of scientific progress: narratives of progress require demonstration, not simply assertion, and they must guard against implications of inevitability. Similarly, I would challenge historians of chemistry to consider critically the ingrained assumptions that the present has no place in accounts of the past (23). Judicious relaxation of such strictures can make accounts produced with historians' skills and attention to context more relevant and interesting to readers outside their own specializations.

When he was President of the American Historical Association, William Cronon gave a measured endorsement to judicious abridgment, at least when historians communicate to a wider public (24):

> Whenever historians seek to make their knowledge accessible to a wider world—whether in books, classrooms, museums, videos, websites, or blogs—they unfailingly abridge, simplify, analyze, synthesize, dramatize, and render judgments about why things happened as they did in the past, and why people should still care today. But they need not commit the worst sins of whiggishness when they do so. The characters in their stories need not wear white or black hats, and will feel more richly human for being understood on their own terms.

Acknowledgment

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3. S. Aspinall, "Don't Judge Historical Figures by Modern Values" (letter), *Financial Times*, Mar. 4, 2021, p 34; retrieved from Gale OneFile: News (accessed April 29, 2021).
4. Scholarly history of any sort is a vastly different mode of portraying the past than the construction of monuments, as was pointed out by a reviewer of this paper, so it may seem odd to introduce an essay on the former by using examples of the latter. I do so partly to illustrate present-day interest in depictions of the past and partly because using present-day considerations in describing the past is directly relevant to the essay.
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11. Quoted from T. S. Kuhn, "History of Science," *International Encyclopedia of the Social Sciences*, Macmillan, New York, 1968, Vol. 14, pp 74-83 on 76-77; quoted in S. G. Brush, "Scientists as Historians," *Osiris*, 2nd ser., **1995**, *10*, 214-231 on 218. Thomas Kuhn (1922-1996) was a Ph.D. physicist whose academic career was primarily in the history and philosophy of science.
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13. L. M. Principe, *The Secrets of Alchemy*, University of Chicago Press, Chicago, 2013, p 137. Principe has doctorates in chemistry and in history of science, and his faculty appointment at Johns Hopkins University is in the departments of chemistry and of history of science.
14. The 1944 report (R. B. Woodward and W. E. Doering, "The Total Synthesis of Quinine," *J. Am. Chem. Soc.*, **1944**, *66*(5), 849) was a "formal" synthesis: the researchers did not themselves produce quinine, but an intermediate whose conversion to quinine had been previously reported in the chemical literature. That conversion was subsequently called into question. An historical investigation marshalled considerable evidence that supported the original claim (J. I. Seeman, "The Woodward–Doering/Rabe–Kindler Total Synthesis of Quinine: Setting the Record Straight," *Angew. Chem. Int. Ed.*, **2007**, *46*, 1378-1413). A year later, an experimental investigation reproducing the questioned steps also supported the original work (A. C. Smith and R. M. Williams, "Rabe Rest in Peace: Confirmation of the Rabe–Kindler Conversion of *d*-Quinotoxine Into Quinine: Experimental Affirmation of the Woodward–Doering Formal Total Synthesis of Quinine," *Angew. Chem. Int. Ed.*, **2008**, *47*(9), 1736-1740).
15. Ref. 11 (Brush), p 215. Stephen Brush earned a Ph.D. in physics. Most of his academic career was in history of science at the University of Maryland.
16. H. Chang, "We Have Never Been Whiggish (About Phlogiston)," *Centaurus*, **2009**, *51*, 239-264. Chang is Hans Rausing Professor of History and Philosophy of Science at the University of Cambridge. Physics is part of his undergraduate education, and his doctorate is in philosophy.
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21. A. M. Silverstein and S. Weinberg, "The Whig History of Science: An Exchange," *New York Review of Books*, Feb. 25, 2016, p 41. A reviewer of the present article wondered what Weinberg would think about, among other things, "absolute space and time, determinism in classical physics, etc." I suspect that he would have described these as limiting cases and not "simply wrong." I would argue that analyzing those concepts in light of both past and current knowledge enriches our understanding of them. But I would argue (with Chang) that the same holds for the phlogiston theory despite Weinberg's implication that it was "simply wrong."
22. D. Alvargonzález, "Is the History of Science Essentially Whiggish?" *Hist. Sci.*, **2013**, *51*, 85-99. Alvargonzález is a philosopher by training. He is professor in the Departamento de Filosofía of the Universidad de Oviedo.
23. Michael Gordin examined the anti-whig orientation of historians of science in an essay review of Hasok Chang's book *Is Water H_2O?: Evidence, Realism and Pluralism* (Springer, Dordrecht, Netherlands, 2012). Gordin writes that "the professional history of science as a discipline is officially and resolutely 'anti-Whiggish,'" and he affirms his commitment to that position. M. Gordin, "The Tory Interpretation of History," *Hist. Stud. Nat. Sci.*, **2014**, *44(4)*, 413-423. Gordin is Professor of History at Princeton University, and his education is in history of science, including an undergraduate concentration in history and science at Harvard.
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REFLECTIONS ON THE LAST AND THE NEXT HUNDRED YEARS

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Abstract

The ACS History Division has fostered a hundred years of fascinating work in the history of chemistry, presented orally and in writing. The following essay offers a series of suggestions of what the future might hold. There is still much to be discovered, celebrated, reinterpreted, and pondered.

The Division of History of Chemistry has come a long way since Charles Albert Browne and Edgar Fahs Smith took a break from attending ACS sessions, and spent a relaxing hour chatting about their mutual historical interests under a stand of trees on Evanston's Lake Michigan shore in September 1920 (1). The two men took steps to begin to organize a new ACS division during the following two semiannual ACS meetings. At the spring 1921 meeting, Browne and Smith sought to convene "all cranks who were interested" in helping to launch such a section; in the fall, they summoned fellow "kindred spirits" together "to discuss their hobbies" (2). The waggish tone implying that the history of chemistry was merely a harmless hobbyhorse of cranks seems a little surprising, considering that Browne and Smith were both educated partly in Germany, which had a long and continuing tradition of sophisticated historical scholarship in history of science, and also considering that both men proved to be thoroughly able historians. However, the tone fit with the early twentieth-century American pattern of purely avocational interest by professionals in the history of their discipline (3). By a generation later the discipline of history of science in the United States had dramatically matured, with the rise of graduate programs and university departments dedicated to the subject. By the 1970s, the authors of a history of the ACS discussed the resulting competition in the History Division between "historians of chemistry" who had been formally trained in the historical discipline, and "chemist-historians" who had come to the subject from chemistry itself. Each of these communities, Skolnik and Reese tactfully and correctly opined, "have crucial roles to play" (4).

The nearly half-century since Skolnik and Reese's assessment has seen further changes, and although I will shortly suggest many compelling reasons for celebration and optimism, it must be said that some recent developments have been disappointing. When I began graduate study more than fifty years ago, there were two highly respected historians of chemistry in the Department of History of Science at the University of Wisconsin, Aaron Ihde and Robert Siegfried. Today there are no historians of chemistry in Madison, and even the department itself no longer exists, the historians of science having been absorbed into Wisconsin's Department of History. This is an example of loss to our field that is paralleled in some other American universities, including my own. Advanced study in the history of the physical sciences has been partly coopted in recent years by the history of bio-medically related fields, and partly displaced by a growing emphasis on the history of the social and human sciences (which is not to suggest that those fields are unworthy of study). Making matters worse is the state of the Ph.D. job market. When I began graduate study, openings were still reasonably plentiful, but by the time I was looking for a tenure-track position the market was already in deep recession, and it has not improved since that time. Even more personally troubling, our field in recent years has lost some of its most eminent members, distinguished scholars and beloved colleagues such as Jim Bohning, George Kauffman, Stan Tarbell, Owen Hannaway, Colin Russell, Larry Holmes, Mel Usselman, David Knight, and Maurice Crosland.

But there is also an abundance of good news. Many younger scholars have successfully braved the headwinds; they are finding positions and are steadily contributing fine new scholarship. The annual production of monographs and scholarly articles in our field continues to increase, as does the number of specialist journals, book series, societies, and conferences. The *Bulletin for the History of Chemistry* and *Ambix* continue to publish papers of the highest quality; indeed, in 2013 *Ambix* successfully transitioned from a triannual to a quarterly journal, with a ca. 33% increase of content and no diminution of quality. *Angewandte Chemie International Edition* continues regularly to publish fine historical papers. Two independent journals for philosophy of chemistry were founded during the 1990s, *Hyle* and *Foundations of Chemistry*, and more recently the history of chemistry celebrated the creation of a new peer-reviewed open access journal, *Substantia*. The "Synthesis" book series of the University of Chicago Press has to date published 19 books on the history of chemistry since its inception in 2010; moreover, there are now two different book series from a single publisher, SpringerBriefs in the History of Chemistry, and Springer's new series entitled "Perspectives in the History of Chemistry." Due to appear next year is Bloomsbury's six-volume multi-author *Cultural History of Chemistry*, charting the development of the science from antiquity to the present—the first multivolume history of chemistry since J. R. Partington's masterwork concluded more than 50 years ago. For the past 30 years the historical group within the European Chemical Society has been organizing stimulating biennial international conferences in the history of chemistry. The Chemical Heritage Foundation in Philadelphia, recently renamed Science History Institute but still devoted principally to the history of chemistry, has grown apace over its nearly 40-year history, and constitutes a scholarly mecca for our field. Another outstanding international focal point for the pursuit of history of chemistry, as well as for other specialties in the history of science, is the Max Planck Institute for the History of Science, founded in Berlin in 1994. These are just some of the markers that indicate the continuing health of our field.

The range and importance of historical studies of the chemical sciences derive directly from the range and importance of chemistry itself. In recent years chemists have sometimes expressed dismay that the very word "chemistry" is used less frequently today to label chemical specialties, departments, and programs, in preference to such words as "molecular biology," "nanoscience and nanotechnology," "macromolecular science," "molecular sciences and engineering," "materials science"—even "molecular biophysics," which leapfrogs verbally right over chemistry, which is at the heart of the molecular, biological, and physical aspects of that field. But there is a sense in which this trend must be more expected and celebrated than lamented, for of all the scientific disciplines it is chemistry, the "central science," that has the most uniquely fuzzy and permeable borders. As a consequence, interdisciplinary efforts that cross those borders, as reflected in the phrases just cited, have a correspondingly wide range of labels from which to choose.

And it is here that we find even more good news. Since chemistry sometimes functions in this way partly as a disciplinary tool-box for neighboring fields, we historians of chemistry have available to us a correspondingly large range of historical topics and approaches from which to choose, a degree of flexibility that is enjoyed by few other branches of history of science. In addition, chemistry is today, and has been throughout history, more closely tied than any other branch of science to material productivity and to industrial, artisanal, and medical fields. This circumstance also opens the historian's door to innumerable kinds of studies that explore the relevance of chemistry to social, cultural, and technological history.

What this means, in turn, is that there is scope for a wide range of new historical studies with a chemical theme. We have barely begun to explore many areas. Probably the most wide-open field of all is the hugely significant and hitherto little explored history of recent chemistry. Such investigations can be done with many different approaches and foci, but relatively few scholars have the technical prerequisites and have braved the intrinsic difficulties in carrying out these kinds of studies. One obvious approach here is to explore in a detailed and technically proficient manner the rise of landmark scientific contributions, as Jeffrey Seeman does with such mastery (5); another type is the skillful interweaving of sociological and institutional history with the actual chemistry, as is admirably exhibited in recent papers by Stephen Weininger (6). We need many more studies of these types, as well as investigations of the cultural, social, technological, and political dimensions of our science in the twentieth (and even the early twenty-first) century. It would be gratifying, and an opportunity seized, if we could see more work from the community of chemist-historians appear in journals that are usually patronized by historians of chemistry, as well as more work by historians of chemistry in chemical journals. Perhaps another means of bridging and unifying these two communities would be to see more published research by co-authored collaborations across that divide, a pattern that to date has been only occasionally seen.

At the other end of the chronological spectrum, we can surely say that the revolution in our understanding of the history of alchemy that has taken place over the last generation only demonstrates how much there is still to learn about early chemistry, chymistry, alchemy, and related artisanal pursuits (7). We have only begun to understand the full scope of chemically-related activity in antiquity and the middle ages, partly because the of the linguistic skills that are needed to carry out such studies—not only Latin and Greek, but also in many cases Arabic, Syriac, or even, for the most distant antiquity, cuneiform Akkadian. Regarding the Latinate and vernacular medieval and early modern worlds, Pamela Smith's multidisciplinary "Making and Knowing" project at Columbia University crosses boundaries between artisanal crafts, chymistry, and early modern epistemologies; similar in some ways is Ursula Klein's program to explore the "ontology of materials" and early technoscience in seventeenth- and eighteenth-century Europe (8). Smith and Klein exemplify another wide-open approach to the history of chemistry, namely pursuing studies that integrate the history of chemistry with philosophy of science. The leading exemplar of this kind of project, mostly applied to a later chronological period, is Hasok Chang's innovative program of "complementary science," which can be carried further in innumerable directions (9).

One can easily construct an arbitrarily extendable list of further relatively open fields for new studies in the history of chemistry. Purely for illustration, here are a few examples: the history of women and underrepresented minorities in chemically-related endeavors; chemistry in "the periphery"—that is, anywhere other than the major European countries from the early modern period on, such as the United States before 1900, south Asia, east Asia, Africa, South America, the Middle East, and European nations whose people speak "minor" languages; chemically related subjects in domestic life and other mostly hidden contexts, such as food production and preparation; the development of laboratories and laboratory apparatus and instruments; the development of chemistry as a discipline; chemistry and war through the ages; mutual interactions with politics and political economy in history; and chemistry and culture, e.g. in relation to the history of literature, music, and fine arts (10). I do not mean to suggest any of that these areas are still devoid, or even close to devoid, of good contributions; fine scholars have produced much excellent work in all eight of these categories. I only mean to indicate that in each case there is still plenty of room for countless additional interesting and important historical investigations. History of chemistry, like the history of science more broadly, is still a relatively young field. For this reason it is much more open, compared to fields of history that have been intensively cultivated (or, using another metaphor, mined) for generations, thus requiring doctoral candidates to be satisfied by ever narrower research projects. That is not our problem.

The areas I know best are naturally those in which I have been active over many years: the development of chemistry in Great Britain, France, and especially Germany during the course of the nineteenth century, with particular attention to the rise and development of the atomic theory and of the field of organic chemistry. By contrast to my illustrative list of eight notably open fields in our discipline mentioned in the previous paragraph, the rise of English, French, and German chemical atomic theory and organic chemistry are subjects that have always been considered to sit at the very heart of the history of chemistry, and so there was already a rich historiography in these subjects before I ever began work as a historian. However, despite this more intensive cultivation by historians—admirable work that extends back well over a century and a half—even here there are innumerable historical questions still to be more fully answered, and countless complex historical puzzles that have not satisfactorily been resolved.

An example is the extraordinary career of Jacob Berzelius, which has often been studied, but rarely examined in the sort of definitive detail that we really would like to see (11). Turning from Sweden to France, I am struck by the extraordinary richness of manuscript sources that have only begun to be fruitfully mined; some collections have scarcely been touched. Despite Maurice Crosland's masterly biography of Gay-Lussac (12), there is much that we still want to know about this extraordinary scientist. Regarding Jean-Baptiste Dumas, who was so powerful a player in French (and pan-European) chemistry that younger contemporaries sometimes jocularly referred to him as “l’être suprême,” we have a variety of important studies, but nothing like what we really need in order to understand his career in all its multifarious detail (13). A partial list of important and interesting figures in the history of nineteenth-century Francophone chemistry whom I consider to be still radically insufficiently studied, especially by Anglophone historians, I would name (alphabetically ordered): Antoine Balard, Marcellin Berthelot, Auguste Cahours, Michel-Eugène Chevreul, Henri Sainte-Claire Deville, Edmond Frémy, Charles Friedel, Charles Gerhardt, Auguste Laurent, Charles Marignac, Alfred Naquet, Jules Pelouze, Jean-François Persoz, Victor Regnault, Jean Servais Stas, and Louis-Jacques Thenard.

This enumeration suggests the richness of what is yet to be explored in a subset of my own already relatively well-worked specialty field, the history of nineteenth-century chemistry; and it should be noted that the list was predicated on just two search terms: “French or Francophone” and “biographical approaches.” A similar abundance of future meaty research topics in the history of nineteenth-century European chemistry can be seen when we turn to other countries, and to other approaches besides biography: internal scientific, cultural, social or sociological, political, institutional, topical, industrial, and so on. Opportunities abound for us and all of our younger and future colleagues of the field.

But why, exactly, do we bother? What is it that draws us to investigate the history of chemistry? I want to suggest five (nonexclusive and often overlapping) reasons.

Certainly one important goal is professional acculturation, education, and elevated status. Chemistry is obviously an occupation for which one trains, but it is also more than that: it is a true profession that demands, and benefits from, proper professional formation. What distinguishes a profession from “a job” is not just deep expertise, but also the associations, the culture, the ethics, the esthetics, the social functions … *and the history* … of the relevant field. Just as attorneys, physicians, clerics, musicians, and visual artists feel themselves to be members of socially significant callings extending back through the centuries, so do (or so should) scientists. In short, the history of chemistry is (or should be) an essential element of what it means to become, and to be, a chemist.

Second, our endeavors offer the means toward a new perspective not just on science of the past, but on our contemporary science, as well. One category of such historical projects are those that provide novel instruction and practical ways to look at the science of today. Hasok Chang has argued that history can play a heuristic role, in regaining lost work, lost methods, and lost perspectives that have present utility. Another category of the multivalent relationship between the old and the new is laboratory replications of landmark historical chemical contributions, which can provide new insights into historical events (14). There is much to learn by following the difficult paths that our forebears have successfully struck through the scientific thickets.

Third, there is inspiration and collective memory to consider. The history of chemistry is a multifarious tale of extraordinary achievements that richly deserve memorialization; it represents our professional heritage, and merits celebration in many ways and forms. This is the formative thought behind two ACS programs, the National Historic Chemical Landmarks and the Citations for Chemical Breakthroughs.

Fourth, a closely related point: history of chemistry illuminates the essential humanity of science—the creativity, imagination, and artistry, along with serendipity, that so often is exhibited by the best science (along with the 99% perspiration about which Thomas Edison rightly spoke). This can be a helpful corrective to the unfortunate image often unintentionally portrayed in textbooks, of colorless automatons mindlessly following a tedious algorithmic scientific method, isolated from their social milieu. The science of chemistry has been created by centuries of efforts by fascinating and (mostly) admirable individuals working in formative historical contexts. Exploration and appropriate portrayal of those individuals and those contexts is vital both for effective science pedagogy, and for the promotion of public appreciation of contemporary chemistry.

Finally, let us never forget the simple pleasures of pursuing and reading history, of whatever kind; done right, it is wonderful fun. As L. P. Hartley famously put it, “The past is a foreign country; they do things differently there;” and in the same way that it is fascinating to visit actual foreign countries, so also it is a special treat vicariously to breathe the air, to view the scenes of daily life, and to witness the labors, disappointments, and triumphs of our predecessors in this endlessly intriguing endeavor we call chemistry.

For all of these reasons, and for the indefinite future, I look forward to the fascinating history that will be revealed in each new issue of the *Bulletin for the History of Chemistry*—as well as in all the other journals that publish papers in our field.

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1. C. A. Browne, "The Past and Future of the History of Chemistry Division," *J. Chem. Educ.*, **1937**, *14*, 503-516 on 504. See also J. J. Bohning, "Looking Back: Eighty-five Years of Chemists and their History," *Bull. Hist. Chem.*, **2007,** *32(2),* 66-81.
2. C. A. Browne and M. E. Weeks, *A History of the American Chemical Society: Seventy-Five Eventful Years*, ACS, Washington, DC, 1952, p 288.
3. R. Laudan, "Histories of the Sciences, and Their Uses: A Review to 1913," *Hist. Sci.* **1993,** *31*, 1-34.
4. H. Skolnik and K. M. Reese, *A Century of Chemistry*, ACS, Washington, DC, 1976, pp 308-309. I write the following thoughts as an academically trained historian; chemist-historians would surely have different and equally legitimate perspectives on these matters.
5. E.g., J. I. Seeman, "The Woodward-Doering/Rabe Kindler Total Synthesis of Quinine: Setting the Record Straight," *Angew. Chem. Int. Ed.*, **2007**, *46*, 1378-1413; J. I. Seeman, "Woodward-Hoffmann's *Stereochemistry of Electrocyclic Reactions*: From Day 1 to the *JACS* Receipt Date," *J. Org. Chem.,* **2015**, *23*, 11632-11671. Peter Morris and Seeman discuss history of recent chemistry in their essay in this issue: "The Importance of Plurality and Mutual Respect in the Practice of the History of Chemistry," *Bull. Hist. Chem.*, **2022**, *47*(1), 124-137.
6. E.g., L. Gortler and S. J. Weininger, "Private Philanthropy and Basic Research in Mid-Twentieth Century America: The Hickrill Chemical Research Foundation," *Ambix*, **2017**, *64*, 66-94; S. J. Weininger, "Delayed Reaction: The Tardy Embrace of Physical Organic Chemistry by the German Chemical Community," *Ambix*, **2018,** *65*, 52-75. Weininger's essay in this issue is about the history of recent chemistry: "'The Poor Sister:' Coming to Grips with Recent and Contemporary Chemistry," *Bull. Hist. Chem.***, 2022**, *47*(1), 119-123.
7. I refer to the works of such scholars as Allen Debus, William Eamon, Bruce Moran, William Newman, Tara Nummedal, Lawrence Principe, and Pamela Smith.
8. E.g., P. H. Smith, *The Body of the Artisan: Art and Experience in the Scientific Revolution*, University of Chicago Press, 2004; U. Klein, *Technoscience in History*, MIT Press, 2020.
9. H. Chang, *Is Water* H_2O*? Evidence, Realism, and Pluralism*, Springer, Dordrecht, 2012.
10. Regarding the interrelations between chemistry and wider culture, or the culture of chemistry itself: in my close involvement with the preparation of the *Cultural History of Chemistry* series mentioned above I was continually struck by how problematical it proved to be to ask chapter authors to remain closely tied to the first word of the series title.
11. There are exceptions to this generalization. For Berzelius's early research on stoichiometry see Evan Melhado, *Jacob Berzelius: The Emergence of His Chemical System*, University of Wisconsin Press, 1981; for his atomic theory, Anders Lundgren, *Berzelius och den kemiska atomteorin*, Almqvist and Wiksell, Stockholm, 1979. Even H. G. Söderbaum's foundational 3-volume biography, *Jac. Berzelius levnadsteckning,* Almqvist and Wiksell, Stockholm, 1929-31, has limitations, only partly for being almost a century old and available only in Swedish. See also Melhado and Tore Frängsmyr, Eds., *Enlightenment Science in the Romantic Era: The Chemistry of Berzelius and its Cultural Setting*, Cambridge University Press, 1992, and Carl Gustaf Bernhard's inimitable *Through France with Berzelius: Live Scholars and Dead Volcanoes*, Pergamon, Oxford, 1985.
12. M. Crosland, *Gay-Lussac: Scientist and Bourgeois*, Cambridge University Press, 1978.
13. The most recent monograph on Dumas—Jimmy Drulhon, *Jean-Baptiste Dumas (1800-1884): La vie d'un chimiste dans les allés de la science et du pouvoir*, Hermann, Paris, 2011—is invaluable for biographical aspects, but not particularly for the history of chemistry.
14. See for example the historical replication pertaining to the first Seeman paper cited in note 5 that was provided by A. C. Smith and R. M. Williamson, "Rabe in Peace: Confirmation of the Rabe-Kindler Conversion of *d*-Quinotoxine into Quinine," *Angew. Chem. Int. Ed.*, **2008**, *47*, 1736-1740. Lawrence Principe and William Newman have published many fine historical investigations using laboratory replications. For another example, and a guide to the literature using this technique, see also M. Usselman, T. Reinhart, K. Foulser and A. Rocke, "Restaging Liebig: A Study in the Replication of Experiments," *Ann. Sci.,* **2005**, *62*, 1-55.

About the Author

Alan J. Rocke is Distinguished University Professor and Henry Eldridge Bourne Professor of History Emeritus at Case Western Reserve University in Cleveland, Ohio, USA. He has published widely on the history of chemistry in the U.K., France, and Germany during the nineteenth century.

The Back Story

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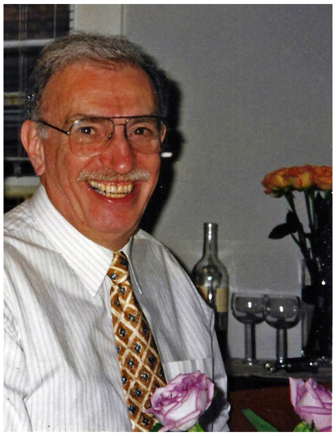
Steve Weininger, Comfortable in Many Disciplines



Stephen J. Weininger is rare among the scholars who pursue the history of chemistry (HoC). His distinctiveness comes in part from his desire and ability to study, publish and present on the history of chemistry for chemists; on the history of chemistry for professional historians; and on the philosophy of chemistry for philosophers. Indeed, he has a particular skill for contributing to these several disciplines simultaneously and is welcome in all three communities. In my first draft of this essay, I included representative titles of Steve's publications, but ultimately that approach seemed too encyclopedic and sterile, the opposite of my intent. Table 1 (in the Supplementary Information) clusters Steve's publications multifurcated by discipline. You are invited to see for yourself his multidisciplinary scholarship.

Regardless of the discipline, Steve publishes in its journals and uses the idiosyncratic style and language of the discipline. He is comfortable in many distinctly different scientific cultures. By formal education and academic appointment, Steve is a chemist. His academic home is in a Department of Chemistry at Worcester Polytechnic Institute (WPI). Steve is a former Chair of the Division of History of Chemistry (HIST) of the ACS. He has published research articles in the *Journal of the American Chemical Society,* the *Journal of Organic Chemistry, Tetrahedron Letters,* the *Journal of Polymer Science*, and so forth. As we shall shortly see, by passion, Steve became a self-educated historian and philosopher of chemistry.

Perhaps Steve's transformation from chemist to interdisciplinarian began in 1970 when WPI revised its curriculum to stress interdisciplinary teaching and research. Steve and others formed a *Group for Integrative Studies*. One course that Steve initiated and eventually taught with a colleague in the Art History Department was *Light, Vision and Understanding*. In the early 1980s, together with like-minded colleagues from other institutions, Steve founded a Society for Literature & Science, now called the Society for Literature, Science, and the Arts (SLSA). Steve was its first vice president and ultimately its president. Still a very active organization, SLSA holds annual conferences and publishes a journal, *Configurations*—a double entendre from the chemist's perspective or perhaps an "in joke" played by Steve on his SLSA colleagues.

I am particularly amused by some of the titles (and what's inside them) in Steve's portfolio. Here are several: "Sooner Silence Than Confusion: The Tortuous Entry of Entropy into Chemistry" (with Helge Kragh) in *Historical Studies in the Physical Sciences* (1996); "Contemplating the Finger: A Semiotic Perspective on Chemistry" in *HYLE* (1998); "Chemistry for the 'Industrial Classes': Laboratory Instruction, Mass Education and Women's Experience in Mid-Western Land-Grant Colleges, 1870-1914" in the *Bulletin for the History of Chemistry* (2013) (chosen for the Best Paper Award by HIST); and "Paper Tools from the 1780s to the 1960s: Nomenclature, Classification, and Representations" (with Mary Jo Nye) in *Ambix* (2018); among others.

How can it be that Steve is welcomed in so many disciplines beyond his home discipline of chemistry? It is his combination of academic brilliance, professional amiability, and personal charm. One of our colleagues said of him, "Steve shows that he cares about you by always giving you his full attention. He's really interested in you and what you have to say." Another colleague said, "Everyone loves Steve. His enthusiasm for chemistry, for scholarship in any field, for food and drink, for fellowship, for life in general, is incredibly infectious. He is kind and thoughtful, but also has a quick, analytical mind. Life is good when you are around Steve."

Steve tells me that his paper in this special issue of the *Bulletin*—aptly focused on bringing the above-named disciplines closer together—will be his last scientific publication. He is hanging up his reins and saddle for the last time. His absence in the post-2022 literature and at our HoC meetings will be keenly felt. Our loss will be tempered with the knowledge that he and his fertile mind will be dancing, along with his wife Jennifer, to other tunes in other venues.

Steve is one of my heroes. I have particularly admired his warm smile, which he offers generously. If one cannot hope to duplicate this virtuoso model, one can surely value and appreciate Steve Weininger.

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