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A Tale of Two Sciences, 1860-1985

Abstract – Episodes in the recent histories of chemistry and physics serve to pinpoint the differences between these two cultures.

Introduction

A very old joke sets the difference between a chemist and a physicist. The chemist, so it goes, makes inaccurate measurements on extremely pure substances, whereas the physicist performs extremely accurate measurements on impure samples. There is a complement: biologists are guilty of inaccurate measurements on extremely impure samples.

There is considerable truth in this witticism. Gabor Somorjai's testimony will suffice [1], "In the early 1960s, it was difficult to be sure that the (platinum (100)) surface was clean. My luck was that I was a chemist rather than a physicist. (...) In the early 1970s the dominance of physics in surface science was almost over. Until then I was the only chemist working with modern techniques using single crystals in surface science – in ultra-high vacuum, for example, to keep the surface clean enough to put molecules onto it."

This joke is my point of departure. It implies, does it not, both a symmetry and a complementarity between the two disciplines, physics and chemistry. Is this true? Does it apply in practice? Does it account for developments in the recent histories of the two sciences?

I shall start the story in the 1860s when the structural theory of chemistry was devised. I shall close it about 1985, just prior to nanoscience and nanotechnology becoming fashionable.

Within those 125 years, what is an appropriate periodization? 1860-1890 was

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the first phase, with the widespread adoption of structural formulae by chemists and the slow rise of stereochemistry [2]. The second period, 1890-1914, encompassed spectacular advances by physicists in the understanding of atomic structure. The third period takes us to 1927, when Walter Heitler (1904-1981) and Fritz London (1900-1954) published their quantitative description of the H₂ molecule. I shall devote an entire section to the period 1927-1932, that of a short-lived idyll between physics and chemistry. The fifth period is the nineteen-thirties, following the discovery of the neutron which recalled to the fold those physicists who had been building a bridge with chemistry. The sixth period, in the aftermath of World War II, ran from 1945 to 1985: physicists had learned their lesson from their collaboration with the military and had become proficient at public relations and money-raising. Chemists, while somewhat envious of the physicists' lobbying skills, were otherwise fully engaged by the second revolution which their science underwent during that period, due in part to nuclear magnetic resonance (nmr), a powerful new tool which the physicists had fashioned for them. This 1945-85 period saw also an erosion of physical chemistry within the pecking order among the chemical disciplines to the profit of synthetic organic chemistry.

The Chemical Bond

This part of the story consists of such well-known episodes that I need only a small reminder of each. It is noteworthy for a simple distinguishing criterion between the two disciplinary communities, chemists and physicists. They did not speak the same language.

During the 1860s, a number of chemists such as August Kekulé von Stradonitz (1829-1896), Alexander Crum Brown (1838-1922), Archibald Scott Couper (1831-1892) devised the structural theory of organic chemistry [3]. In this basically heuristic scheme, a molecule was represented by a structural formula. The atoms were connected by dashes or lines in this graphical depiction. The number of such lines depended on whether the connexion was of the single, double or triple bond type.

These organic chemists – who little worried about a proof for the actual existence of the atoms – had developed structural theory as a shorthand. It was coherent. It accounted for a vast corpus of observations, and it was predictive. In the words of Ira Remsen (1846-1927), who thus summarized what was then the majority opinion [4], “The formulas are but the condensed expressions of the conclusions which are drawn from the reactions.” Starting with Le Bel's and van't Hoff's 1874 proposal of a tetrahedral carbon atom, structural formulae became tridimensional – a gradual development which took place over the last decades of the nineteenth century. Structural formulae partook of a spirit both empirical and pragmatic. The nature of these chemical bonds remained opaque. This did not get in the way of organic chemistry moving on rapidly.

At about the time when stereochemistry blossomed, physical chemistry came on the scene. It was the brainchild of Wilhelm Ostwald (1853-1932) [5]. While organic structural formulae treated atoms and atomic theory with at worst benign neglect, Ostwald's initial position was exclusion. He would not let the subdiscipline he had just created be contaminated by atomic ideas. This excommunication lasted until 1906, when he had to eat his words. By that time however, physical chemistry had immunized itself against recourse to microscopic structures as explanations. It consisted near-exclusively of thermodynamics [6] and kinetics.

Physical chemistry became a specialized area within chemistry, one of its sub-disciplines. Only within chemistry? Why not within physics also? Because physics at the very moment of the inception of physical chemistry was intent upon investigating atomic structure rather than denying it.

Physical chemistry was beset with this original sin. An accurate and perceptive summary was made by Neville Vincent Sidgwick (1873-1951) in 1931, when a visiting Baker Lecturer at Cornell [7]:

“It is a remarkable sign of the predominance of the thermodynamic aspect at this time that Ostwald actually proposed to abandon the ideas of atoms altogether. (...) By the irony of fate, this doctrine of Ostwald's was propounded exactly at the time when the physicists began their triumphant attack on the problem of the structure of the atom.”

Irving Langmuir (1881-1957) had earlier made the same point, Ostwald's legacy had left physical chemistry with a blind spot, which still endured by the time when Langmuir made these remarks towards the end of the 1920s [8]:

“Under the leadership of Ostwald, chemists began to adopt a much more critical attitude and began to distinguish carefully between what they considered experimental facts and hypotheses based upon these facts. Ostwald, although he recognized the convenience of the atomic theory, believed it must always remain impossible to prove the existence of atoms or molecules. He therefore urged that chemists avoid as far as possible the use of such hypotheses. Perhaps the chief result of this attitude was to lead physical chemists to neglect those parts of chemistry where the atomic theory would have been most helpful and to devote themselves more specially to the fields in which energy relationships and thermodynamics were directly applicable. (...) The progress of physical chemistry was probably set back many years by the failure of the chemists to take full advantage of the atomic theory in describing the phenomena that they observed. The rejection of the atomic theory for this purpose was, I believe, based primarily upon a mistaken attempt to describe nature in some absolute manner” [9].

Indeed, physicists discovered the electron at the time of the birth of physical chemistry. And during the early years of the twentieth century, following the discoveries of X-rays and radioactivity, work proceeded briskly on atomic structure. The physicists, led by Ernest Rutherford (1871-1937), Max Planck (1858-1947) and Niels Bohr (1885-1962) among others, evolved a planetary model for the atom, with a central nucleus and orbiting electrons. The orbits were connected via quantum

numbers to spectroscopic lines for the elements, previously grouped empirically into series (Balmer, Lyman, Paschen, ...). Needless to say, these structural advances by physicists were expressed in equations. Ever since Galileo made his celebrated pronouncement [10], math had been the master tool for advances in physics.

Not in chemistry though. Chemists were allergic to mathematics [11, 12]. At the same time, the turn of the twentieth century, when atomic structure was elucidated, chemists in their vast majority did not feel concerned. Why should they care? They had their own structural theory. While physicists struggled to understand atomic structure, chemists had under their belts more than a generation-worth of empirical studies of molecular structure.

Chemists were not ignorant though and they followed with acute interest the progresses in atomic physics, such as the discovery of the electron. They were quick to integrate it into their doctrine [13]. In 1916, Gilbert Newton Lewis (1875-1946) published his major paper, in the *Journal of the American Chemical Society*, on “The Atom and the Molecule” [14]. He argued there that

“the type of union which we have so far pictured, although it involves two electrons held in common by two atoms, nevertheless corresponds to the single bond as it is commonly used in graphical formulae.”

To reach such a conclusion, which led to the introduction of what came to be known as Lewis formulae, Lewis resorted to his encyclopaedic knowledge of chemical compounds of many types, both ionic and nonpolar. His argument avoided mathematic equations entirely. It is qualitative and, to some extent, iconic (the cubical atom).

There are strong, positive reasons for scientists to organize themselves into specialized communities. These provide professional societies and peer-reviewed journals, plus a whole system of quality control, from the granting of degrees and of research monies to the awarding of prizes. Disciplinary identity buttresses itself both with guiding concepts (inclusionary) and avoidance notions (exclusionary).

Disciplinary conformism, usually fierce, compares with nationalistic chauvinism. Scientists, who otherwise might feel isolated from operating on the frontier of knowledge, gain a compensating sense of belonging to a (sub)disciplinary mainstream. Hence, there is a perceived need for a few among one’s fellow-scientists to act as go-betweens. They bring foreign epistemic objects into the mainstream and make them look indigenous. G.N. Lewis was such an interpreter when he introduced the notion of the chemical bond as an electron pair. He allowed chemists to preserve their earlier structural language as the guiding concept. He simultaneously let them avoid learning the new quantum ideas and the new atomic physics.

We move now to the following decade, the nineteen-twenties [15]. By 1927, Friedrich Hund (1896-1997) and Robert S. Mulliken (1896-1986) had introduced their molecular orbital or MO theory [16, 17]. Couched in the language of mathematics, this was a theory aimed at physicists, not at chemists [18]. The same year,

another two physicists, who also resorted to mathematical description, published their theory of the dihydrogen molecule [19]. As Henry Frank commented not long afterwards [20],

“When a physicist ... succeeds in showing that his theoretical model of the atom makes it necessary that two hydrogen atoms shall unite to form a molecule, while two helium atoms cannot do so, the chemist is interested. This is not very startling information, to be sure, but its *mathematical incorporation* into the general body of physics is new and significant” (emphasis added).

These developments did not impact chemists, who continued to rely on Lewis structural formulae [21, 22]. The chemical community waited until 1931 for one of its members, Linus Pauling, to publish his epochal paper on “The Nature of the Chemical Bond.” Pauling’s approach was a popularization of the new quantum mechanics. Since he addressed fellow-chemists, his language was as much purged of mathematics as he could get away with. Pauling served as the interpreter to chemists of the new quantum physics.

His Baker Lectures at Cornell University, published in 1939 in the book by the same title [23], capping a series of papers on this topic, also more or less closed the structural phase of Pauling’s career, as he moved on to the next phase, the study of biological molecules and processes. He brought to bear in that book his extensive knowledge of chemical structure, based on numerous X-ray and electron diffraction studies [24]. Publication of that book, followed by that of textbooks, of *General Chemistry* in particular, turned the valence bond (VB) theory promoted by Pauling into the orthodox language of structural chemistry. Organic chemists in particular would not resort to the MO description until the 1950s and the promotion of MO theory by a few militants, such as Charles A. Coulson (1910-1974) [25], Jack Roberts (1918-) [26], and Andrew Streitwieser (1927-) [27, 28]. During the whole period 1940-1960, VB theory reigned supreme among organic chemists worldwide due to a large extent to Pauling’s prestige. Of course, VB theory benefited from what one might term the “nested Russian dolls” asset of many scientific theories. Pauling’s valence-bonds integrated Lewis formulae which in turn encompassed the earlier structural theory from the 1860s, to which Kekulé’s name is associated foremost.

Physical Methods of Chemistry

One might describe chemistry by its tools. If one indeed does so, they come under two categories. The more ancient, which chemists inherited from their predecessors, whether alchemists, assayers and smelters, apothecaries, glassmakers, varnishers, potters, ... include alembics, retorts, pelicans, crucibles, phials and glassware of many types. The more recent date to Lavoisier’s reliance on the most accurate scales which could be devised in his time. I note in passing that Lavoisier liked to view himself more as a physicist than as a chemist.

After the balance, the next addition to the list of physical instruments [29, 30] was Biot's polariscope, introduced during the 1830s. There were other additions to the chemists' armentarium during the second half of the nineteenth century, especially after Bunsen and Kirchhoff had invented spectroscopy.

But the explosion in the number and diversity of physical tools in the chemical laboratory occurred in the aftermath of World War II [31]. Infrared and UV-visible spectrometers, X-ray and electron diffractometers (following Linus Pauling's lead), gas phase and liquid phase chromatographs, ultracentrifuges, mass spectrometers, electron spin resonance and nuclear magnetic resonance spectrometers, chiroptic instruments for optical rotatory dispersion and circular dichroism, ...

A first take on the phenomenon, too naive, is to describe it as a contribution from physics to chemistry. In this view, the latter discipline is indebted to the former for a cornucopia of instruments it has thrived upon.

This is simplistic. Chemists were not passive recipients of those techniques. They developed methodologies without which use within chemistry of those tools would have been severely limited. Scientists active at the interface of physics and chemistry, responsible for the chemical applications, were often chemists. The physical methods of chemistry should not be viewed as a colonial theater of operations for physics. To a large extent, chemists actively imported them from physics and, more importantly, devised the operational procedures.

Consider some actual examples. Case number 1 is the polariscope. It measures the angle of rotation of polarized light by a liquid sample. Devised by the physicist Jean-Baptiste Biot (1774-1862) in the 1830s, its design was improved by a succession of instrument makers. It became more or less stabilized in the 1880s. This instrument then remained invariant for a century or so, until the laser replaced other light sources, such as the sodium flame which the Bunsen burner made possible in the 1860s.

It was chemists, though, who turned the polariscope (or polarimeter, as it was also named from its inception) from a demonstration to a research instrument. True, Biot the physicist had discovered sucrose inversion. However, the chemist Augustin-Pierre Dubrunfaut [32] explained sucrose inversion by its hydrolysis into glucose and fructose [33]. The chemist Ludwig Ferdinand Wilhelmy (1812-1864) reported in 1850 the mass action law which, he found, ruled the sucrose inversion reaction [34]. And Wilhelm Ostwald (1853-1932) published in 1884 his study of sucrose inversion, as catalyzed by a variety of acids. He used this reaction as a probe into acid strength [35], thus laying a cornerstone of physical chemistry.

The thermodynamics and kinetics of sucrose inversion became emblematic of physical chemistry, as shown by the sucrose inversion experiment monitored by the polarimeter which generations of students performed during the twentieth century [36]. Likewise, the polarimeter became emblematic of organic chemistry from an altogether different application. Pasteur in 1860 [37, 38, 39, 40] showed that organic molecules as a rule were chiral and characterized by their specific optical rotation.

Case number 2 is nuclear magnetic resonance. A key episode in its history was the discovery, made by W.G. Proctor and F.C. Yu, of the so-called chemical shift [41, 42]. Chemists did not lag behind, Herbert S. Gutowsky (1919-2000) was quick to rise to the occasion [43].

The chemical shift rapidly became an essential feature in the determination of chemical structure using nmr. The irony is for its very name to have been introduced at the time when the age-old distinction between chemical and physical properties became obsolete and was jettisoned, even from elementary textbooks of general chemistry. As a further irony, the *chemical* shift is quite obviously a *physical*, not a chemical property, if one goes by the operational definition, according to which determination of a *chemical* property affects the basic nature of the substance.

Advocates of the paternalistic colonial viewpoint, claiming a progressive and civilizing influence of physical methods, cultural imports from physics into chemistry, would find support in the relegation to the dustbin of history of the distinction between chemical and physical properties, if indeed its demise were the consequence of the massive penetration of physical methods in chemistry.

Just as with the polarimeter, chemists adopted the nmr spectrometer as a black box with a throughput function. The input was a chemical sample. The output was a chemical structure. The nmr spectrum, rather than the nmr spectrometer, was the new device to incorporate into the eclectic toolbox of the chemist.

A Blossoming

Rather than focusing in the usual way on the Schrödinger-Heisenberg quantum mechanics, with its chemical fallout, I shall concentrate here on its periphery. During the short period of 1927-32, physicists made an incursion into chemistry, and they were of the first rank. Their foray, for although short-lived, nonetheless left durable and important results. In many ways, those physicists jump-started entire subdisciplines, most notably chemical physics.

Max Born (1882-1970) and Julius R. Oppenheimer (1904-1967) suggested their approximation in 1927 [44]. Michael Polanyi (1891-1976), jointly with Eugene Paul Wigner (1902-1995) and Henry Eyring (1901-1981), formulated the original theory of the transition state for chemical reactions between 1925 and 1931 [45, 46]. Henry Eyring would during the 1940s become the interpreter for physical chemists of this novel theoretical framework. He expressed transition state theory in the existing language, that of thermodynamics and kinetics.

John von Neumann (1903-1957) and E.P. Wigner published their theorem in 1929 [47]. Llewellyn Hillel Thomas (1903-1992) and Enrico Fermi (1901-1954) the previous year published their theory, a description of the electron density in a molecule [48, 49]. Not to forget the already mentioned calculation of the hydrogen molecule by Heitler and London, in 1927. Crystal-field theory appeared in 1929

from Jean Becquerel (1878-1953) [50] and Hans Bethe (1906-2005) [51], to be further developed by Hendrick Anton Kramers (1894-1952) [52] and, later on during the 1930s, by John Hasbrouck van Vleck (1899-1980) [53].

This last example, crystal-field theory is exemplary of how much these pioneers were ahead of the pack. Their effort to a large extent was premature. Only after World War II would ligand-field theory blossom from the seed planted by Hans Bethe and his colleagues a couple of decades earlier [54].

A few other comments are in order. One may conjecture a reason for the attractiveness of chemical questions to physicists. I submit that it was the time of a lull in atomic physics, in-between periods of intense activity. Indeed, the foray into chemistry was all over by 1932 [55]. The reason for the hasty retreat was very simple. The neutron had been discovered. Physicists rushed back to the fold and studied nuclear structure with gusto and intense competitiveness.

Most of these momentous strikes into the chemical field occurred in Germany. Most of the publications appeared in German journals. The rise of the Nazis in 1933 would shatter the pre-eminent role of German institutes and physicists.

The contributions to chemistry I have evoked came in the language of mathematical equations. There was very little overlap with chemical language. The chemists meanwhile, as I have pointed out, were intent upon preserving their autonomous formulations such as Gilbert Newton Lewis's cubical atoms [56].

Physicists brought their training and their mentality to bear on questions in chemistry. Their need for a focused and formalized conceptualization expressed itself in the devising of a master equation, whether with respect to the relationship of electronic energies to a wavefunction (Schrödinger), to the relative motions of electrons and nuclei (Born-Oppenheimer) or within transition state theory.

There was thus a need for an intermediary space, one for a dialog between the two disciplines, an in-between zone where physics and chemistry could mutually benefit each other. The interdisciplinary chemical physics filled that void. It also served as a bulwark, as a buffer zone: pure physics would not be contaminated by a chemical approach, pure chemistry – organic chemistry in particular – would remain immune from math and from chemical physicists.

Chemical physics was needed, because it was out of question to use physical chemistry for this interdisciplinary purpose. It became durably tarred by its initial hostility (Ostwald's) to atomic theory. It continued to be heavily influenced by its traditional concerns, thermodynamics and kinetics. The first issue of the *Journal of Chemical Physics* appeared in January 1933. It marked the official beginnings of the new subdiscipline [57, 58].

Comparing Themselves to Physicists

Language reveals major differences between the two sciences. Consider just the two adjectives, *physical* and *chemical*. The physical sciences, if one is to heed

the *Oxford English Dictionary*, deal with inanimate matter, as opposed to the biological sciences, or the moral sciences. To resort to more contemporary language, the physical sciences are demarcated from the biological sciences and from social studies [59].

Just note the nonreciprocity. Chemistry is part of the physical sciences. But physics does not belong to the chemical sciences. Physics is more encompassing if we are to believe this cursory look at ordinary language. This first linguistic rule applies in many languages besides English and French. The expression, physical sciences, is about two centuries-old in both these languages. Implicit in it is the reductionist claim, chemistry is reducible to physics, to which I shall return.

There is a second rule. The expression, the chemical industry, is standard. Conversely, one does not speak of the *physical industry** even though this is a well-formed locution. One may talk about the electronic industry or the automotive industry, but not about the physical industry. While chemistry is both a science and an industry, physics is taken to be only a science – even though it can boast of industrial applications too numerous to mention.

This striking dissymmetry between the two adjectives, chemical and physical, underscores an underlying prejudice, which goes back to Greek antiquity, to Plato and Aristotle. To study physics is noble, it is an aristocratic pursuit. Conversely, to study chemistry is synonymous with dirtying one's hands. Physics engages the mind, it is a predominantly intellectual pursuit; while chemistry is a mere craft, which indeed is derived historically from the activities of smelters, apothecaries, distillers, makers of stained glass, jewelers and assayers. Physics, in this view – exaggerated for the purpose of the argument – belongs in the study. Chemistry belongs in the workshop. Physics, to stick with such stereotypes, has no odor. Chemistry not only smells, it stinks.

It is extremely interesting to note that such notions, crude to say the least, have endured for at least several centuries. If indeed the distinction in language between the chemical and the physical goes back to social prejudice against manual work, deeming intellectual pursuits superior, could one not, so goes the counterargument, rule it out as obsolete? “What about the laboratory?”, one wants to argue. Is it not the common workplace of chemists and physicists alike?

The reference to the laboratory is indeed well-taken. But, as soon as we start investigating this notion, the physics-chemistry duality jumps back at us with a vengeance. An historian of physics may declare that one of Galileo's foremost contributions was to invent the laboratory in the seventeenth century. This totally overlooks the fact, which most historians of chemistry are all too well aware of, that the laboratory existed for several centuries before Galileo's time. Alchemists devised it, as part of their protocol for ensuring that their procedures were reproducible, performable under controlled conditions in apparatus devised and built for this purpose. Roger Bacon (c1214-1292) is a much better candidate than Galileo (1564-1642) as inventor of the laboratory.

I now return to the issue of reductionism, one of the sticks with which physicists – some physicists, to be fair – beat chemists. Its most famous (or infamous) expression was the sentence by Paul A.M. Dirac (1902-1984) at the beginning of his paper on the quantum mechanics of many-electron systems:

“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are [now] completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble” [60].

The ensuing issue, that of reductionism, even though it has had no practical impact whatsoever, has nurtured a whole cottage industry among philosophers of science. I shall content myself here with the witty rejoinder by Hugh Christopher Longuet-Higgins (1923-2004), who, going along a reverse path to that of reductionists, derived a bit of math from chemistry [61, 62].

Which brings up the battle for funding with the rival discipline, physics. Physicists in the 80s were better than chemists at grantsmanship, at public relations and were henceforth more successful in getting mammoth collective projects financed. The Pimentel Report (PR), published in 1985 in the U.S. by the National Academy of Sciences as one of its leitmotifs is noteworthy for repeated comparison between the two disciplines, to the effect that physics is enjoying greater financial support than chemistry by the Federal agencies in the US [63]. Chemists, conversely and as also illustrated in the PR, prided themselves on demographics, on beating physicists in sheer number of jobs – or better yet in production of Ph.D. scientists [64].

Chemists, as exemplified by PR, pride themselves in the number of graduate students and Ph.D.s in their discipline. Any drop, as at the time of writing, is perceived as ominous. What are their arguments, in their promotion of chemistry to students having to choose between careers?

The Insistence on Low-Tech

A standard promotional argument by a chemist aiming at recruiting students in the laboratory is to indirectly stress the low-tech characteristics of the research. “You can have an idea in the morning, devise an experiment to test it in the afternoon, and take home the answer in the evening,” goes the argument. Just as with the joke referred to at the beginning of this paper, it carries truth.

It would be an oversimplification to summarize under the heading of “Big Science” [65] the equipment of the chemical laboratory during the nineteen-fifties and – sixties, with expensive instruments, such as chromatographs and spectrometers. One could make a case for the resilience of the notion of “chemistry as craft:” evidence in support would be, for instance, the recourse to thin-layer, paper or column chromatography in complement with gas or high-pressure liquid chromatographies. The former, low-tech tools requiring a measure of dexterity and of care in their use, turned out to be as important to the daily life of the laboratory as

the latter, high-tech methods. Accordingly, before the Golden Sixties [66] came to an end chemists to some extent could see themselves with a foot in each of the two worlds, that of traditional chemistry, basically unchanged for two or three centuries, and that of modern chemistry, with a plethora of new and powerful physical methods at their fingertips [67].

The A-60 was the instrument of change. Built in Palo Alto, California, by Varian Associates, it was a hands-on, routine instrument which graduate students in chemistry could operate themselves. Precalibrated charts, together with an internal lock on a water sample tube, allowed for a single sweep to record a spectrum [68]. The A-60 brought nmr to the masses. Chemists took to it like a fish to water [69].

I claim the A-60 as a low-tech tool. James Shoolery and Varian Associates meant it as a routine instrument, aimed at chemists. To use it was no more involved than using a polarimeter. We come full circle with such a comparison, since chemists found out fairly quickly the ability of the nmr spectrometer to replace a polarimeter, even for its emblematic application, viz. determining the optical purity of a reaction product.

The nmr tube replaced the test tube. The assertion echoes that by Victor Hugo when he claimed so perceptively in *Notre Dame de Paris*, in the superb *ceci tuera cela* digression, that when Gutenberg invented movable type, the book killed the cathedral and its imagery which had been so important earlier in educating Christians.

For centuries, chemists were associated with test tubes, not only in the popular imagination. The test tube was used primarily for qualitative analysis. Adding a few drops of a reagent would trigger a response, maybe a color change, a turbidity or a precipitation. The chemist would then infer the likely presence of a component in the liquid mixture, be it a ketone or sulfate anions.

With the nmr tube, chemists were offered a lighter and more subtle perturbation. The reagent now consisted only of radiofrequencies (RF). Their resonant absorption by the sample in the nmr tube yielded a comprehensive inventory of the groups of atoms present. The nmr tube did not directly replace the test tube, it came on the heels of spectroscopic cells, as had been used in electronic absorption (uv-visible) or in vibrational (ir and Raman) spectroscopy.

Moreover, nmr was revolutionary for a *Gestalt* switch (to borrow Kuhn's phraseology) in perceptions by chemists. Earlier on, molecules were identified by their functional groups, carbonyls, hydroxyls and the like, which were like beacons (as reflected in chemical nomenclature, in its affixes and priorities). Now, especially at the beginning of the nmr era (Fifties and Sixties) when ^1H nmr thrived by itself, not yet complemented by ^{13}C nmr, what shone instead through a spectrum was the hydrocarbon skeleton.

Matter, when under a magnet and tickled by RF waves, gained meaningfulness. Nmr was a microscope of a different order. It displayed inter-relationships between atoms in a molecule [70]. Couplings among nuclei, whether scalar or

dipolar couplings, were the silk threads in the spider web which the nmr spectrum revealed. Nmr truly was the Ariadne's thread guiding chemists to their Holy Grail of structural elucidation.

I single out Jack Roberts for the role of interpreter, bringing in nmr from physics (and the chemical industry) into chemical science.

The web of interactions thus revealed in turn mapped molecular structure. Spectral analysis (the nmr tube) had replaced chemical analysis (the test tube). Analyzing a spectrum, furthermore, was an exact science, not an interpretation fraught with uncertainty, open to skepticism and dispute. True, the nmr spectrometer was an instrument devised by physicists. However, it did not carry with it an interpretative language. Nmr spectra could be read through the usual filter, that of the traditional Lewis chemical formulae.

Conclusion

This paper started with the contention that chemistry and physics are sister sciences, symmetrical and complementary in spirit and methodologies. From the preceding, we have to conclude that such an assumption is untenable.

Let me summarize the evidence, in ten points or so. Firstly, it is rather remarkable that there have been very few scientists who qualified as both physicists and chemists. Lavoisier (1743-1794) was assuredly one of them, Faraday (1791-1867) another. One may wish to add to this short list the names of Ampère (1775-1836) and of Johann Josef Loschmidt (1821-1895). However, who else qualifies during the period of interest, 1860-1985? Only a handful of scientists: Marie Curie 1867-1934) arguably, the Braggs, William (1862-1942) and Lawrence (1890-1971) who bridged the two disciplines, Peter Debye (1884-1966) assuredly, who held successive appointments in physics and in chemistry. This observation in itself suggests a deep divide between the two disciplines.

A second point is both psychological and sociological. It goes back to the origins of both sciences in the early modern period. Physics is aristocratic in nature, while chemistry is plebeian. The former is more of an intellectual quest, the latter is more of a manual craft.

Thirdly, the two sciences differ in their material culture, high-tech in the one, low-tech in the other.

Fourth, they differ in their modes of representation. Physics uses mathematical equations. Chemistry uses an iconic language, that of the structural formulae. The symbols differ, they are algebraical in physics, geometrical in chemistry.

Fifth, the two sciences contrast in their basic urges. Physics is normative and legalistic, where chemistry is inherently transgressive [71, 72].

Sixth, they differ in their defining activities. The physicist measures and builds models, the chemist sets-up and monitors transformations, following which he or she purifies the products.

Seven, the two sciences differ in their unifiers. Chemistry sees itself as a combinatorial art. Physics sees itself more as the work of reason, as the epitome of rationality. Towards the end of the 1945-85 period, quantum chemistry offered itself as the unifying description, i.e., in the role which thermodynamics had played a century earlier.

Eight, the two sciences take different views of matter, points in a force field for the one, substances for the other [73].

Nine, they have different agendas. Physicists seek natural laws, while chemists content themselves with rules.

And, ten, they differ in their focus. Where physics is integrative, chemistry privileges the specific.

Thus, my overriding conclusion is that the two professions differ widely, in language, in objectives, in their methods and in outlook. To refer to them as sister sciences is a stereotype, carrying little validity.

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- [6] At the turn of the twentieth century, thermodynamics (as perfected Boltzmann and Clausius among others) seemed to offer a joint language to chemists and physicists. For a couple of decades indeed, it had a unifying role and an interdisciplinary impact. Gibbs's rule was seen as a master equation, of almost metaphysical status to someone like Henry Adams, as a representative of the educated layman: Adams, Henry. *Mont Saint Michel and Chartres*. Penguin Classics, Harmondsworth, Middlesex: Penguin Books, 1986 (1904); Adams, Henry. *The Education of Henry Adams*. Oxford World Classics, Oxford: Oxford University Press, 1999 (1906).
- [7] Sidgwick, N.V. "The relation of physics to chemistry." *Science* 73 (N° 1889 (Friday, March 13) 1931): 269-276.
- [8] Langmuir, Irving. "Modern concepts in physics and their relation to chemistry." *J. Am. Chem. Soc.* 51 (October, N° 10 1929): 2847-2868.
- [9] Ostwald was not alone in his stand against atomic theory. He had distinguished company. In Germany, Ernst Mach (1838-1916) objected to it too, from his outlook as a positivist. In France, Marcelin Berthelot (1827-1907) opposed it for similar reasons. Likewise, the younger Henry Le Chatelier (1850-1936) fought atomic ideas while his contemporary and successful competitor in ammonia synthesis, Fritz Haber (1868-1934) espoused them.
- [10] Galileo. "The Assayer." In *The Controversy on the Comets of 1618*, Philadelphia: University of Pennsylvania, 1960 (1616).
- [11] Simões, Ana and Kostas Gavroglu. "Issues in the History of Theoretical and Quantum Chemistry, 1927-1960". In *Chemical Sciences in the 20th Century*, ed. C. Reinhardt. 51-74. Weinheim: Wiley-VCH, 2001.
- [12] While there is a whole active field of mathematical physics, there is nothing comparable in chemistry – not much anyway. Alexander T. Balaban has taken exception to such a statement of mine in Laszlo, Pierre. "Circulation of Concepts." *Foundations of Chemistry* 1 (1999): 225-239. For his views, see Balaban, Alexander T. "Reflections about mathematical chemistry." *Foundations of Chemistry* (2005): 1-18.
- [13] Hughes, W. "A possible reconciliation of the atomic model of Bohr and of Lewis and Langmuir". *Nature* 110 (1922): 37-38.
- [14] Lewis, Gilbert N. "The Atom and the Molecule." *Journal of the American Chemical Society* 38 (1916): 762-786.
- [15] Walker, James. "The role of the physicist in the development of chemical theory." *J. Chem. Soc.* 121 (1922): 735-745.
- [16] Hund, F. Z. *Physik* 36 (1926): 657.
- [17] Mulliken, Robert S. *Phys. Rev.* 32 (1927): 186.

- [18] Simões, Ana and Kostas Gavroglu. "Issues in the History of Theoretical and Quantum Chemistry, 1927-1960." In *Chemical Sciences in the 20th Century*, ed. C. Reinhardt. 51-74. Weinheim: Wiley-VCH, 2001.
- [19] Heitler, W. and F. London. *Z. Physik* 44 (1927): 455.
- [20] Frank, Henry S. "Chemistry and the new physics." *Lingnan Soc. J.* 8 (1929): 605-617.
- [21] Some chemists attempted merging the traditional description and the discoveries by the physicists, in their teaching too. See for instance Blanchard, W.M. "Role of valence and of electrons in the teaching of general chemistry." *Proc. Indiana Acad. Sci.* 37 (1927): 245-253; Fry, H.S. "A pragmatic system of notation for electronic valence conceptions in chemical formulas." *Chemical Reviews* 5 (1928): 557-568.
- [22] Robert Robinson (1886-1975) adopted Lewis structures. In the early nineteen twenties, he complemented those formulae with curly arrows to denote movement of electrons in pairs: Kermack, William Ogilvy and Robert Robinson. "An Explanation of the Property of Induced Polarity of Atoms and an Interpretation of the Theory of Partial Valences on an electronic Basis." *Journal of the Chemical Society* 121 (1922): 427; Robinson, Robert. *J. Soc. Chem. Ind.* 43 (1924): 1297.
- [23] Pauling, Linus. *The Nature of the Chemical Bond and the Structure of Molecules and Crystals: An Introduction to Modern Structural Chemistry*. Ithaca, NY: Cornell University Press, 1939.
- [24] Hoffmann, Roald, Sason Shaik, and Philippe Hiberty. "A Conversation on VB vs MO Theory: A Never-Ending Rivalry?" *Accounts of Chemical Research* 36 (10 2003): 750-756.
- [25] Coulson, C.A. *Valence*. Oxford: Oxford University Press, 1952.
- [26] Roberts, J.D. *Notes on Molecular Orbital Calculations*. New York: W.A. Benjamin, 1961.
- [27] A. Streitwieser, Jr. *Molecular Orbital Theory for Organic Chemists*. New York: John Wiley and Sons, 1961.
- [28] It had been known since the nineteen-thirties that both descriptions, VB and MO, would extrapolate to equivalence for a polyatomic molecule.
- [29] Kempf, Richard. "The practical value of physical apparatus and methods in the progress of the natural sciences." *Chem.-Ztg.* 52 (1928): 649.
- [30] Klopsteg, P.E. "Physical methods and measurements in chemistry." *Can. Chem. Met.* 15 (1931): 131-133.
- [31] In 1942, the arsenal of physical instruments for chemists was still limited only to the balance, the pH-meter, IR and UV spectrometers, X-ray and electron diffractometers, mass spectrometers and electron microscopes. See Killefer, D.H. "Physical tools in chemistry." *Rev. Sci. Instruments* 13 (February 1942): 49-53.
- [32] Hewitt G. Fletcher, Jr. "Augustin-Pierre Dubrunfaut – an early sugar chemist." *Journal of Chemical Education* 17 (153 1940).
- [33] Dubrunfaut, A.P. "Note sur quelques phénomènes rotatoires et sur quelques propriétés des sucres." *Compt. Rend. Ac. Sci. Fr.* 23 (1846): 38-44; Dubrunfaut, A.P. "Sur une propriété analytique des fermentations alcoolique et lactique, et sur leur application à l'étude des sucres." *Ann. Chim. Phys.* 21 (1847): 169-178.
- [34] Wilhelmy, L.F. "Ueber das Gesetz, nach welchem die Einwirkung der Säuren auf den Rohrzucker stattfindet." *Annalen der Physik und Chemie* 81 (1850): 413-428, 499-526, 527-532.
- [35] Ostwald, W. "Studien zur chemischen Dynamik. III. Die Inversion des Rohrzuckers." *J. Prakt. Chemie* 29 (1884): 385-408.
- [36] Physical chemistry continued to run on its impetus during that whole century, under its original program dominated by kinetics and thermodynamics, avoiding the infusion of quantum chemical ideas by relegating theoretical chemistry into a narrow corner.
- [37] Pasteur, Louis. *Leçons de chimie professées en 1860*. 1861.
- [38] Ladenburg, A. "Synthese der activen Coniine." *Deutsch. Chem. Gesellsch.* 19 (1886): 2758-2583; Ladenburg, A. "Synthèse de la conicine." *Comptes-Rendus Ac. Sci. Fr.* 103 (1886): 876-880.

- [39] Landolt, H. *Das Optische Drehungsvermögen Organischer Substanzen und dessen Praktische Anwendungen*. 2nd ed., Braunschweig: F. Vieweg und Sohn, 1898; Landolt, H. and J. McRae. *Optical Activity and Chemical Composition*. London: Whittaker, 1899; Landolt, Hans, O. Schönrock, P. Lindner, F. Schütt, L. Berndt, and T. Posner. *The optical rotating power of organic substances and its practical applications*. 2nd ed., Easton, PA: Chemical Publishing Company, 1902.
- [40] Appelquist, J. "Optical activity: Biot's bequest." *American Scientist* 75 (1 1987): 59-68.
- [41] Proctor, W. and F.C. Yu. *Physical Review* 77 (1950): 717.
- [42] There was precedence for the phrase: Knight, W. *Physical Review* 76 (1946): 1259; Bloembergen, N. *Physical Review* 75 (1947): 1326; Dickenson, W. *Physical Review* 77 (1950): 736.
- [43] Gutowsky, H.S. and C.J. Hoffman. *Journal of Chemical Physics* 19 (1951): 1239; Meyer, L., A. Saika, and H.S. Gutowsky. *Journal of the American Chemical Society* 75 (1953): 4567.
- [44] Born, M. and R. Oppenheimer. "Zur Quantentheorie der Molekeln." *Ann. Phys. (Leipzig)* 84 (1927): 457-484.
- [45] Polanyi, M. and E. Wigner. *Z. Physik.* 33 (1925): 429.
- [46] Eyring, H. and M. Polanyi. *Z. Phys. Chem.* B12 (1931): 279.
- [47] Neumann, J. von and E.P. Wigner. *Physik. Zeitschr.* 30 (1929): 465.
- [48] Thomas, L.H. "The calculation of atomic fields." *Proc. Camb. Phil. Soc.* 23 (1927): 542-548.
- [49] Fermi, E. "Un metodo statistico per la determinazione di alcune priorietà dell'atome." *Rend. Accad. Naz. Lincei* 6 (1927): 602-607.
- [50] Becquerel, J.Z. *Physik.* 58 (1929): 205.
- [51] Bethe, H. *Ann. Physik* [5], 3 (1929): 133.
- [52] Kramers, H.A. and J. Becquerel. *Proc. Acad. Sci. Amsterdam* 32 (1929): 1190; Kramers, H.A. *Proc. Acad. Sci. Amsterdam* 33 (1930): 953.
- [53] Vleck, J.H. van. *Theory of Magnetic and Electric Susceptibilities*. 1932.
- [54] Ballhausen, C.J. "History of the Crystal Field Approach." In *Introduction to Ligand Field Theory*, ed. C.J. Ballhausen. 2-6. New York: McGraw-Hill, 1962.
- [55] It occurred with full awareness of its timeliness, Semkovskii, S. Yu. "Physics and chemistry as sciences." In *Trans. VI Mendeleev Congr. Theoret. Applied Chem.* in *Trans. VI Mendeleev Congr. Theoret. Applied Chem. 1932, 2 Part 1* 83-109 (1935) Year.
- [56] Clark, G.L. "Introductory remarks in the symposium on atomic structure and valence." *Chemical Reviews* 5 (1928): 361-364.
- [57] Nye, Mary Jo. *From Chemical Philosophy to Theoretical Chemistry. Dynamics of Matter and Dynamics of Disciplines 1800-1950*. Berkeley: University of California Press, 1993.
- [58] Physical chemists perceived chemical physics as a rival sub-discipline, as some kind of an upstart. Physical chemists held on tightly to their position at the interface of physics and chemistry. See for instance Lange, Erich. "Inquiry into the boundaries of physics, chemistry and physical chemistry." *Sitzber. Physik.-med. Sozietät Erlangen* 65 (1934): 73-94; Holleck, Ludwig. "Physical chemistry and chemical technique." *Z. Ges. Naturw.* 5 (1939): 148-151. Others were calling for a merging of the two sciences, see Wise, Harold. "An integration of physics and chemistry." *J. Chem. Ed.* 20 (1936): 68-72.
- [59] For a very long time and well into the twentieth century, the physical sciences were equated with the experimental. See for instance Boys, C.V. "Physical science and the art of experiment." *Nature* 100 (1918): 477-478.
- [60] Dirac, P.A.M. "Quantum mechanics of many electron systems." *Proceedings of the Royal Society of London* A123 (1929): 714-733 (the sentence occurs on p. 714).
- [61] Longuet-Higgins, H.C. "An application of chemistry to mathematics." *Scientific Journal of the Royal College of Science* 23 (1953): 99-106.
- [62] Superconductivity is a good example of a physical phenomenon not easily reducible to equations: "In 1956, I heard probably the greatest of all calculators, Dick Feynman, declare pub-

- licly that he had calculated the best he knew how and could not find any behaviour resembling superconductivity – and he was only the best of the many brilliant physicists including Einstein and Heisenberg who had tried.” Anderson, P.W. “Emergence, reductionism and the seamless web: When and why is science right.” *Current Science* 78 (6 (25 March) 2000): 1-4.
- [63] 1985, *Opportunities in Chemistry*, National Academy of Sciences, Washington, DC.
- [64] A statement to be balanced with the disaffection of undergraduate students for the sciences, for chemistry in particular, starting in the Seventies: Neckers, D.C.: 1979, “On the Quality of Undergraduate Students Choosing Chemistry as a Profession 1961-1979. A Report.”, Department of Chemistry, Bowling Green State University, Bowling Green OH 43403, also referred to in *Chemical and Engineering News*, Dec. 17, 1979.
- [65] Weinberg, A.M.: 1967, *Reflections on Big Science.*, MIT Press, Cambridge, MA.
- [66] A representative example is that of the University of North Carolina, in Chapel Hill: Burse, M.M. and Crockford, H.D.: 1982, *Carolina chemists: sketches from Chapel Hill*, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC, especially p. 209.
- [67] Physical organic chemistry, as a sub-discipline, embodied such a duality. In the hands of leaders such as J.D. Roberts or J.A. Berson, it synthesized the molecules it needed for physical measurements. See, for a survey of the mechanistic role of the physical organic philosophy the paper by Hine, J.: 1960, May 9, “Physical Organic Chemistry”, *Chemical and Engineering News*, 101-106.
- [68] Anon. “Low Cost, Simple Operation Expand NMR Uses.” *Chemical and Engineering News*, 1961, 52-53.
- [69] Jackman, Lloyd M. “NMR in Organic Chemistry – the Fabulous Fifties.” In *Encyclopedia of nuclear magnetic resonance*, eds. David M. Grant and Robin K. Harris. 397-298. 1. Chichester: Wiley, 1996.
- [70] Barton, D.H.R.: 1972, “The principles of conformational analysis (Nobel lecture 1969)”, in: Nobel Foundation (eds.), *Nobel Lectures. Chemistry 1963-1970*, Elsevier, Amsterdam, p. 309.
- [71] Bensaude-Vincent, Bernadette. *Faut-il avoir peur de la chimie?* Paris: Les Empêcheurs de penser en rond, 2005.
- [72] This difference alone pits the two cultures in opposition. I am reminded of another contrast between two cultures, all too familiar to me. In the United States, “to be a regular kind of guy” is a positive and even laudatory statement. In France, to say of someone “*c’est une personne très ordinaire*” is a highly pejorative statement.
- [73] Gabriel-François Venel (1723-1775) had already drawn attention to this distinguishing mark: Venel, Gabriel-François. “CHYMIE”. In *Encyclopédie ou dictionnaires raisonné des sciences, des arts et des métiers...*, ed. Denis Diderot and Jean d’Alembert. 409. 3. Neuchâtel, Paris, etc.: 1753.