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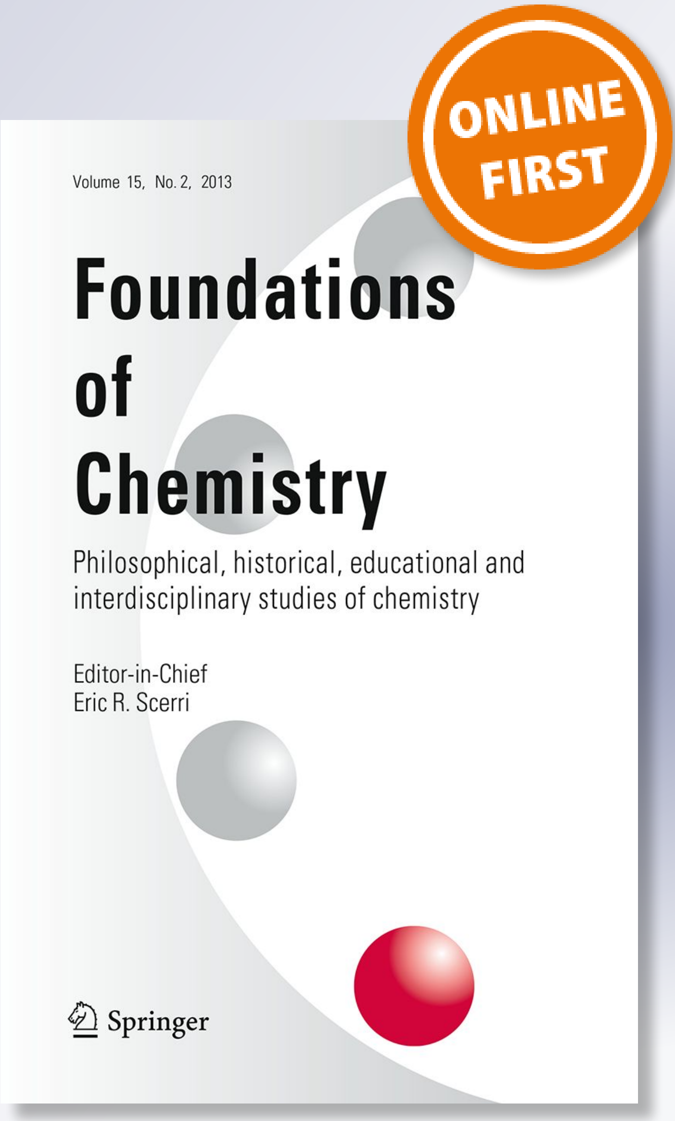

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About continuity and rupture in the history of chemistry: the fourth chemical revolution (1945–1966)

José A. Chamizo[1]

Abstract A layered interpretation of the history of chemistry is discussed through chemical revolutions. A chemical revolution (or rupture, discontinuity, transition) mainly by emplacement, instead of replacement, procedures were identified by: a radical reinterpretation of existing thought recognized by contemporaries themselves, which means the appearance of new concepts and the arrival of new theories; the use of new instruments changed the way in which its practitioners looked and worked in the world and through exemplars, new entities were discovered or incorporated; the opening of new subdisciplines, which produced, separated scientific communities. The fourth chemical revolution, fundamentally characterized by the incorporation of new instruments in chemical practices is discussed.

Keywords Chemical revolution · Emplacement revolution · Layered history · Exemplars · Instruments · Chemical entities

Introduction

> Whereas chemistry is inherently innovative, enriching itself with novel products and with novel routes to known products, its teaching is too often conservative, based on reproduction of what one was taught. It is only necessary to peruse textbooks and their table of contents to realize that chemistry teaching (1) is highly repetitious, shying away from renewal; (2) lags years if not decades behind the front lines in the advancement of chemical science (Lazlo 2013, p. 1677).

In 1952, almost a decade before the publication of Kuhn's *The structure of scientific revolutions,* the book entitled *The Chemical Revolution. A Contribution to Social Technology*

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appeared. The authors, A. Clow and N. Clow, chose that title to indicate the lack of attention that the development of chemical manufactures had had in the history of the Industrial Revolution. This absence of chemistry and its industry from the narrative of scientific development was not new then, as it is not now.[1] Nowadays, particularly in chemical education, we are confronted with what has been called hidden or crouching chemistry (Talanquer 2010, 2013), and one of the possible reasons for this qualification is the way in which we teach normal school chemistry.[2] For example, years ago, researchers in science education indicated:

> Perhaps the greatest obstacle to incorporating history into chemistry lessons is convenient access by practising teachers to resources that can efficiently teach them the salient history behind scientist and their discoveries. Making an accurate history of chemistry more accessible to teachers is difficult to achieve. A faithful distillation of an admittedly complex history of events or a succession of models into a memorable form and in a suitable grain size for use by practising teachers is a formidable challenge (Wandersee and Griffard 2002, p. 32).

In spite of how conservative chemistry teachers are, as Lazlo indicates in the epigraph, one way to approach the above is through explicitly teaching the history of chemistry.[3] Here I attempt to show one of the ways history of chemistry can be taught.[4] Therefore, following Jensen's initial proposal (1998b), I reconstructed the history of chemistry in terms of five revolutionary moments. That represents a difficult equilibrium between over-simplification and over-elaboration. Initially, these moments are considered through an extended Kuhnian notion of 'paradigm' which enables the incorporation of instruments and sub-disciplines as well as entities, into the revolutionary process and provides an adequate interpretation of such periods of development and consolidation. I have previously discussed these revolutions with different depth (Chamizo 2011, 2014b, 2015, 2017a, b). However, in this paper I consider a broad and more philosophical way of approaching chemical revolutions using the fourth one as an example.

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[1] There are, however, some exceptions like: Friedman and Nordman (2006), Mallar et al. (2009), or (Spangenburg and Moser 2004).

[2] About this Van Barkel et al pointed: All current school chemistry curricula have a dominant substantive structure, based on corpuscular theory, which is rigidly combined with a specific philosophical structure, *educational positivism, and a specific pedagogical structure, initiatory and preparatory training of future chemists* (Van Berkel et al. 2000, p. 127).

[3] About the importance and the ways of teaching history, Husbands recognized: *We need to establish a more subtle, less absolutist understanding of the way in which knowledge is created. Our knowledge of the world and the language with which we describe it is not simply in our own heads, nor is it a given feature of the world in which we are living. It needs to be developed through the process of inquiry in classroom, by teachers and learners in classrooms working to create meanings. Historical enquiry is not to be cut off from personal experience, nor is to be locked into personal experience. It is fundamentally a way of relating the internal, the personal to the external, the public.* (Husbands 2003, p. 64). About teaching history and philosophy of science see Matthews (2014).

[4] For example, by recounting, in a laboratory textbook, the history of chemistry through ten experiments (Chamizo 2010) or following the sequence of the five revolutions indicated here (Chamizo 2018) or using models (Chamizo 2014a).

About continuity and rupture in the history of chemistry

> Too often philosophical debates about the reality of particular entities[5] focus on specific conditions that are taken as defining what counts as "real". By focusing less on definitional aspects and more on the evolution of properties and ideas within a conceptual/physical framework, our philosophical arguments will gain historical accuracy and hence greater credibility as an explication of scientific practice (Morrison 2004, p. 446).

After having coined important concepts as 'revolutions',[6] paradigms[7] and 'incommensurability',[8] Kuhn's ideas about continuity and ruptures in the history of science have been deeply studied and challenged like his lack of interest in technology and laboratory practice.[9] However, ever since James B. Conant in his 1957 foreword to Kuhn's *Copernican Revolution* identified Kuhn's enterprise as pedagogically exemplary, all these concepts have become practically ubiquitous in any discussion of the development of the sciences.

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[5] The entity here is spin.

[6] About the revolution concept, the German historian R. Koselleck indicated: *The semantic content of the word "revolution" is thus by no means unambiguous. It ranges from bloody political and social convulsions to decisive scientific innovations; it can signify the whole spectrum, or alternatively, one form to the exclusion of the remainder…[…]… In other words, Revolution assumes a transcendental significance; it becomes a regulative principle of knowledge, as well as of the actions of all those drawn into revolution. From this time on, the revolutionary process, and a consciousness which is both conditioned by it and reciprocally affects it, belong inseparably together. All further characteristics of the modern concept of revolution are sustained by this metahistorical background* (Koselleck 2004, pp. 44–50).

[7] About the paradigm concept the French sociologist P. Bordieu said: *Paradigm is the equivalent of a language or a culture, it determines the questions that can be raised and those that can be excluded, what can be thought and what is unthinkable; being at the same time an acquisition and a starting point, it represents a guide for future action, a research program to be undertaken, rather than a system of norms. From there the scientific group is so far from the outside world that it is possible to analyse many scientific problems without taking into consideration the societies in which scientists work.* (Bourdieu 2001, p. 34).

[8] At the end of his career Kuhn himself reconsider his earlier conclusions recognizing a different meaning for incommensurability indicating that the emergence of new sub-disciplines within a discipline as a result of a scientific revolution, and accepted by new textbooks, separated scientific communities. Particularly, he recognized that incommensurability is important for the growth of scientific knowledge because it isolates practitioners' communities by creating communication barriers that promote the proliferation of specialities: *First, the episodes that I once described as scientific revolutions are intimately associated with the ones I've here compared with speciation. It's at this point that the previously mentioned disanalogy enters, for revolutions directly displace some of the concepts basic in a field in favour of others, a destructive element not nearly so directly present in biological speciation. But in addition to the destructive element in revolutions, there's also a narrowing of focus. The mode of practice permitted by the new concepts never covers all the field for which the earlier one took responsibility. There's always a residue (sometimes a very large one) the pursuit of which continues as an increasingly distinct speciality. Though the process of proliferation is often more complex than my reference to speciation suggest, there are regularly more specialities after a revolutionary change than there were before…The second component of the return to my past is the specification of what makes these specialities distinct, what keeps them apart and leaves the ground between them as apparently empty space. To that the answer is incommensurability, a growing conceptual disparity between the tools deployed in the two specialities. Once the two specialities have grown apart, the disparity makes it impossible for the practitioners of one to communicate fully with the practitioners of the other. And those communication problems reduce, though they never altogether eliminate, the likelihood that the two will produce fertile offspring* (Kuhn 1992, pp. 19–20).

[9] See for example: Lakatos and Musgrave (1970), Toulmin (1972), Suppe (1979), Gutting (1980), Laudan (1984), Cohen (1985), Hull (1988), Rouse (1998), Dyson (1999), Bourdieu (2001), Baird (2004), Hoyningen-Huene (2008), Chang (2011), Kindi and Arabatzis (2012), Hacking (2013), Marcum (2015), Blum et al. (2016) and Scerri (2016).

In the Postscript to the 1970 edition of *The Structure of Scientific Revolutions*, Kuhn indicated that he had conflated two conceptually distinct connotations of paradigms-'exemplars' and 'disciplinary matrices':

> (…) [b]ecause the term [paradigm] has assumed a life of its own… I shall here substitute 'exemplars.' By it I mean, initially, the concrete problem-solutions that students encounter from the start of their scientific education, whether in laboratories, on examinations, or at the ends of chapters in science texts… All physicists, for example, begin by learning the same exemplars: problems such as the inclined plane, the conical pendulum, and Keplerian orbits; instruments such as the vernier, the calorimeter and the Wheaststone bridge.

Thus, the term 'exemplar' represents a collection of solved problems for a specific historical community, which are generally found in their professional literature, and especially in their textbooks. It is narrower than paradigm and avoids some of the ambiguities that the latter has acquired. Making explicit the role of instruments in normal science reduces the gap between normal and revolutionary science. This has an important consequence, because exemplars, being more flexible and also more practically accurate than paradigms, not only recognize the conceptual or theoretical changes within a discipline, but also indicate that they are accompanied by the design, construction and use of certain instruments.[10]

Paraphrasing Kuhn: an exemplar is what the members of a scientific community share, and conversely, a scientific community consists of men and women who share certain exemplars. Exemplars integrate in different proportions theory and practice.[11] This means that since exemplars are a substantial part of textbooks,[12] they allow that scientific community to communicate to its practitioners what it is considered valid as an explanation. As Woody recognized:

> Textbook exemplars aim to cultivate communal skills and techniques by a more direct, and yes, implicit, form of communication. Skills are introduced by direct demonstration. Correct theory applications is cultivated through mimicry and experience. The original challenge presented by the interpretative gap is not eliminated, but since the exemplars are, by decree, examples of correct application, the challenge is now limited to new cases (Woody 2002, p. 27).

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[10] *There are various ways to approach the study of scientific instruments and their place within the scientific enterprise. With the 'pragmatic turn' in the 1990s, scientific practice, experiments, and instruments increasingly came into focus within the history of science. In many instances, collections, whether public or private, provide the starting point for much current work on scientific instruments.* (Taub 2009, pp. 339–340).

[11] Because the community will judge novel explanations based on their acceptance by practitioners, it is essential these folks be well-trained, reliable judges of explanatory norms…Exemplars, in other words, display without explicitly articulating, what a scientific community judges to be explanatory, what model of intelligibility it has chosen to embrace (Woody 2002, p. 24). Related to exemplars, it has also been indicated: It is tacit knowledge to be sure, but consisting nevertheless of ideas (Wise 2012, p.579).

[12] About the importance of textbooks in science education see: Bensaude-Vincent (2006), or Matthews (2014).

Textbooks exemplars are introduced and accepted socially, and in many cases they are the means through which new entities are incorporated into a scientific community.[13] The history of chemistry is dotted with these stabilized hidden entities,[14] some of which have generated important discussions within the various chemical communities such as phlogiston (Chang 2012), atoms (Bensaude-Vincent 1999), ions (Earley 2005; Goodwin 2013), or between diferent disciplines communities as is the case of the electron.[15] Even more, as Chang pointed:

> Historical epochs are marked out by epistemic objects (entities that we identify as constituent parts of reality) just as much as by people, institutions or theories, so where we recognize continuities and discontinuities in epistemic objects does affect our historiography in substantive ways (Chang 2011, p. 424).

Continuities and discontinuities are the central issue of Kuhn's *The Structure of Scientific Revolutions*. However, after the accumulation of anomalies (problems that resisted solutions by the accepted methods used by a particular scientific community), paradigm shifts (as gestalt switches) were never as complete as the original definition suggested.[16] Kuhn himself later recognized (Kuhn 1992) that incommensurability is important for the growth of scientific knowledge because it isolates practitioners' communities by creating communication barriers that promote the proliferation of specialities. Contrary to popular views, that means, that after a revolution the rupture is not absolute. Theoretical discontinuities conceal underlying continuities at the deepest methodological level, where the disciplinary side of exemplars, that is to say the instruments and the experiments (Holmes and Levere 2000; Chamizo 2013), have their own place. Hence, it is possible to consider that 'chemical revolutions' are emplacement-revolutions, rather than replacement-revolution.[17] They change the way science is practiced without necessarily abandoning all the previous theories or disciplinary tasks.

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[13] *Textbooks are fundamentally conservative as they are meant for training students in solving the puzzles raised within the paradigm* (here the exemplar) *rather than inventing new problems. Kuhn argued that they assume their conservative function through various ways. They present only established and incontrovertible knowledge, the stable results of past revolutions* (Bensaude-Vincent 2006, p. 669).

[14] I agree, following Arabatzis, with the term hidden entities, he said: I have chosen the term "hidden entities" instead of other more familiar terms, such as "unobservable entities" or "theoretical entities", for the following reasons. First, I wanted to avoid the thorny issues surrounding the observable unobservable distinction…Second, I also avoided the term "theoretical entities" because it conveys the misleading impression that hidden entities do not transcend the theoretical framework in which they are embedded. In fact, these entities are trans-theoretical objects, which cut across different theories or even entire disciplines…… […]… a hidden entity might be defined as the object of a body of knowledge and of a set of practices (Arabatzis 2008, p.1, 8).

[15] *As we have seen, however, in other respects the electron's chemical personality and its physical personality diverged considerably. The laws it was supposed to obey (Coulomb vs. non-Coulomb), its putative behavior inside the atom (dynamic vs. static), and some of the properties attributed to it (nonmagnetic vs. magnetic, classical vs. quantum) differed across disciplines* (Arabatzis 2006, p. 199).

[16] Kuhn was faulted for his emphasis on theory, however he recognized since the beginning the importance of experimental procedures. For example about chemistry he wrote: Furthermore, though he (the chemist) may previously have employed them differently, much of his language and most of his laboratory instruments are still the same as they were before. As a result, postrevolutionary science invariably includes many of the same manipulations, performed with the same instruments and described in the same terms, as its prerevolutionary predecessor (Kuhn 1962, pp. 129–130).

[17] One of the referees asked if this is particular to chemistry. The only case that I know that discusses a revolutionary change specifically in these terms, emplacement instead of replacement, is that of the quantum revolution (Schweber 2016). The issue deserves more investigation.

As it was recognized by S. Toulmin, many years ago:

> We can see, now, how the distinction between theoretical and disciplinary considerations enables us to escape the paradoxes of the classical revolutionary view. It may well be that no proposition within Einstein's theoretical physics can be strictly translated into Newtonian terms, or vice versa; yet this fact by itself does not impose any 'rational discontinuity' on the science. On the contrary: when two scientific positions share similar intellectual aims and fall within the scope of the same discipline, the historical transition between them can always be discussed in 'rational' terms, even though their respective supporters have no theoretical concepts in common. Radical incomprehension is inescapable, only when the parties to a dispute have nothing in common even in their disciplinary ambitions. Given the very minimum continuity of disciplinary aims, scientist with totally incongruous theoretical ideas will still, in general, have a basis for comparing the explanatory merits of their respective explanations, and rival paradigms or presuppositions—even though incompatible on the 'theoretical' level—will remain rationally commensurable as alternative ways of tackling a common set of 'disciplinary' task (Toulmin 1972, p. 126).

Thus, we can understand the dynamics between continuity and ruptures using the metaphors of the layers (Elwick 2012). This metaphor allows multiple conditions of possibility from strata: 'higher' strata are made possible by 'lower' ones. It is important to insist that a lower layer does not cause a higher one, but instead makes it possible,[18] as can be seen in Fig. 1.

In the same direction P. Galison's book *Image and Logic* about twenty century physics, differentiated three layers, or levels, of this science: theory, experiment and instrumentation. Discussing the long-term stability of physics, he recognized that there were breaks and revolutions, either in the instrumental, experimental or theoretical domains. The layers are intercalated and each one has different time' spans. Whereas one of them has disrupted, the structures of the other layers remain largely intact.[19]

Thus, through exemplars it is possible to gather both theory and practice of a scientific discipline. Exemplars are particularly useful in chemistry, because chemistry has a long experimental tradition. Furthermore, the historical development of scientific disciplines can be represented by layers, and not necessarily the rupture of one of these layers represents the rupture of the other.[20] In other words, 'chemical revolutions' are

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[18] The stratigraphical metaphor makes easier our description of relationships of dependence and independence between different levels of conditions of possibility. It acts as a shorthand. Thus we usually find strata-talk used to discuss conditions of possibility (Elwick 2012, p. 622).

[19] *When a radically new theory is introduced, we would expect experimenters to use their best-established instruments, not their improvement ones…Examples of the survival of experimental practices across theoretical breaks are now abundant in the new literature of experiment. For the first time there are a real interest in the dynamics of experiment outside the provision of data to induce, confirm, or refute specific theories* (Galison 1997, pp. 799–800). Another physicist F. Dyson adds: *Kuhn saw science from the point of view of a theoretical physicist, taking the experimental data for granted and describing the great leaps of theoretical imagination that enable us to understand. Galison sees science from the point of view of an experimental physicist, describing the great leaps of practical ingenuity and organization that enable us to acquire new data. Although I am a theoretist, I happen to find Galison's views of science more congenial* (1999, Kindle edition loc 220).

[20] For example as Lombardi and Pérez-Ransanz addressed: *If it were shown that quantum mechanics is wrong, it would not affect chemical knowledge about molecular structure, chemical bond or chirality* (Lombardi and Pérez-Ransanz 2012, p. 204).

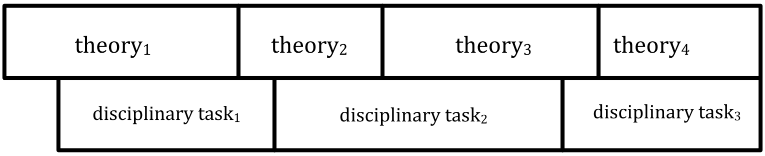

Fig. 1 A layered interpretation of the history of chemistry. In some periods the same disciplinary task, or in our case chemical practice, shares two different theories or one theory can explain two different disciplinary tasks. Sometimes both change at the same time

emplacement-revolutions, rather than replacement-revolution.[21] This means that not all previous concepts are abandoned, but that they are transformed from within, trough shifting the questions being asked and the criteria for acceptable answers, thereby changing the way in which chemistry is practiced. As Humphreys said:

> Replacement revolutions are the familiar kind in which an established way of doing science is overthrown and a different set of methods take over. Emplacement revolutions occur when a new way of doing science is introduced which largely leaves in place existing methods. The introduction of laboratory experimentation was an emplacement revolution in the sense that it did not lead to the demise of theory or of observation (Humphreys 2011, p. 132).

Moreover, as the hidden entities can be incorporated either from the theory or practice, it is in the exemplars where a large part of the disciplinary knowledge is condensed in a certain historical moment. And by doing so, the chemical community stabilizes those hidden entities.[22] In addition, a way to recognize a revolutionary process is to identify the rise of new subdisciplines.

What has been said here basically coincides with Baird (2004) as he indicated that the analytical instrumental revolution, here called fourth chemical revolution, which will be developed below, can be better understood through the characterization of the scientific revolutions of I. Hacking. About them recently, Schweber[23] indicated:

> Hacking Type (HT) revolutions amalgamate pure and applied concerns. They transform a wide range of scientific practices and are multidisciplinary, with new institutions being formed that epitomize the new directions. These "new" institutions can however be "old" ones that have been restructured. The time scale of HT revolutions is the longue durée, but the durées have become shorter as the scientific community

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[21] As Bird stated about replacement revolutions: *Revolutions are primarily changes in theoretical beliefs* (2000, p. 86), what it means here, in only one of the layers.

[22] As Kuhn observed in 1952 and Kim explained in 2014: *chemical atomism requiered a belief in the endurance of elements in their compounds and the recognition of analysis and synthesis as fundamental tools of the working chemist* (Gyung Kim 2014, p. 118).

[23] As an example of scientific revolution he used the quantum revolution: *Considering a "big" scientific revolution such as the quantum revolution as a Hacking-type revolution allows for greater continuity with previous knowledge; it emphasizes the interdisciplinary aspect of the growth of knowledge and makes the social, sociological, cultural and the epistemological an integral part in the historical inquiry. It also considers the limits of the new knowledge and what it entails, which demarcates the revolution. Such a view challenges us to be better historians, yet recognizes the special character of being a historian of science* (Schweber 2016 p. 343).

> has increased. HT revolutions are linked with substantial social change, and after an HT revolution, there is a different feel to the world…HT scientific revolutions that are of particular interest have an additional feature: they make use of a characteristic language to formulate, corroborate, self-authenticate and self-stabilize the style of reasoning it introduced (Schweber 2016, pp. 342–343).

Summarizing, a chemical revolution, as an emplacement revolution, means that after its consolidation, new exemplars are added in the new textbooks. These exemplars recognize the utility of new instruments and introduce new stabilized hidden entities.[24] Moreover new subdisciplines appear and…there is a different feel to the world.

The fourth chemical revolution (1945–1966)

> In the second half of the twentieth century, chemistry underwent a profound transformation. Its object of examination, the chemical substance, was transmuted into abstract structure; its most important method, the chemical reaction was supplemented by physical methods; and its practitioner, the chemist, was partially displaced by technical instruments. At the center of this transformation were physical methods (Reinhardt 2006a) preface.

One of the ways to identify a rupture in the history of chemistry is to recognize the incorporation of new instruments, which accompanied by the consolidation of new entities allows the emergence of new sub-disciplines. The above does not follow a linear ordering and usually happens around a theoretical dispute. In the first revolution with phlogiston' replacement, in the second with the replacement of Berzelius' unique electrochemical model of chemical bond and in the third with the replacement of Dalton's compact atom. In Table 1 there are indicated some of the characteristics of the four chemical revolutions. The first three have already been discussed at length (Chamizo 2014b) however it is relevant to make some clarifications about the dates:

- The Scottish J. Black perfected the analytical balance and in 1754 isolated carbon dioxide from magnesium carbonate in which it can be recognized as the first quantitative chemical reaction. In 1818 the Swedish J.J. Berzelius published the paper "Essai sur la théorie des proportions chimiques et sur l'influence chimique de l'electricité" until then the greater list of atomic weights and its model of electrochemical combination.
- In 1828, Wohler converted ammonium cyanate into urea. In 1874 Independently the Dutch J.H. van't Hoff and the French J. Le Bel explained optical isomerism considering the asymmetry of the carbon atom in these compounds.
- In 1887 W. Ostwald and J. van't Hoff founded the still existing one, *Zeitschrift für Physikalische Chemie*, the first journal devoted to physicochemistry. In 1923, 1 year after F.W. Aston received the Nobel Prize in Chemistry, G.N. Lewis published *Valence*

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[24] About them, and particularly about spin see the epigraph of this section or consider the approach of Kim: *Chemical theories in history did not (perhaps still do not) function in the way histories of theoretical physics and their revolutions dictate. Their task is not to represent nature as it always has been, but to engender a coherent chemical reality that can be made relevant to the representation of nature and society. The world chemist sought to make and describe has not been the immutable 'nature' at least for some time* (Gyung Kim 2014, p. 133).

Table 1 Characteristics of chemical revolutions

Revolution	Main protagonists	Main instruments	Entities	Disciplines and subdisciplines
First 1754–1818	Black, Cavendish, Dalton, Lavoisier, Volta	Pneumatic through, balance, calorimeter	Atom	Chemistry
Second 1828–1874	Berzelius, Cannizaro, Le Bel, Liebig, Mendeleiev Pasteur, van't Hoff, Wholer	Kaliapparat polarimeter	Molecule	Organic chemistry
Third 1887–1923	Aston, Curie, Lewis, Ostwald Thomson, Rutherford	Cathode rays tube, Mass spectrometer	Electron Nucleus	Physical chemistry, Nuclear chemistry
Fourth 1945–1966	Martin, Mulliken Pauling, Perutz, Synge Tiselius Woodward, Zavoisky	Chromatograph, EPR, UV, IR, ^{1}HNMR, X-ray crystallography	Spin	Instrumental analytical chemistry, Theoretical chemistry, Molecular biology

> *and the Structure of Atoms and Molecules* and with M. Randall *Thermodynamics and the Free Energies of Chemical Substances*, while J.J. Thomson *The electron in chemistry.*

The fourth chemical revolution is fundamentally characterized by the incorporation of new instruments in chemical practices. Four Chemistry' Nobel Prizes and one Physics' Nobel Prizes were awarded by research done using new instruments.[25] This rupture in traditional chemical practice has been widely recognized, either as a revolution in itself (Morris 2002) or as an important transformation. The chemistry historian U. Klein said so recently:

> Therefore, I'll restrict my paper to early modern and modern chemistry, say, from the early eighteenth century to the mid twentieth century. I neither include alchemy before ca. 1700 nor the late modern chemistry after ca. 1940. After ca. 1940 quantum chemistry was firmly established and physical spectroscopic instruments and methods of chemical analysis began to proliferate; these changes affected the key epistemological and methodological role played by material substances in all chemical fields until that time. I call the period and type of chemistry that replaced alchemy and predated late-modern chemistry the ''classical chemistry'' (Klein 2012, p. 8).

In 1945 at the end of World War II, the president of the National Science Foundation of the United States, V. Bush, published a report known as *Science. The infinite frontier,* in which he openly requested that the federal government finance science research in American universities and also support the companies that had supplied materials and equipment to the army. With this proposal, which was carried out, chemical laboratories changed more than in the previous 300 years (Prelog 1991; Grasselli 1992). That same year, the foundations of the instrumental technique called electronic paramagnetic resonance (EPR) are established.[26] A few years later nuclear magnetic resonance (NMR) was also established.[27] Both instrumental techniques detect the spin of subatomic particles.

From that moment (Reinhardt 2001; Morris 2002; Lazlo 2006) are introduced or generalized in chemical practices the use of: electrophoresis and ultraviolet visible and infrared spectrometers; X-ray crystallography; the mass spectroscopes (particularly since 1956) and soon, the most important of all, those of nuclear magnetic resonance (Reinhardt 2006a). On the other hand, chromatographs[28] and even the rotary evaporator occupied a place in

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[25] In chemistry: A.W.K. Tiselius in 1948; A.J. Martin and R.L.M. Synge in 1952; M.F. Perutz and J.C. Kendrew in 1962; D.C. Hodgkin in 1964. In Physics to E. Purcell and F. Bloch in 1952, and also in Chemistry, year's later but for the fundamental research done in this period to R.R. Ernst in 1991.

[26] Results of the work of the soviet scientist E.K. Zavoisky.

[27] *Shortly after the end of the war, Bloch and Purcell, each with a small group of collaborators, would observe nuclear magnetic resonance in bulk matter, now referred to simply as NMR. They aimed, in particular, at detecting the resonance signals from protons. Although the magnetic moments were embedded in a rather complex environment, compared to the case of essentially isolated atoms or neutrons in previous experiments, the apparatus needed for these measurements was much simpler. In an interesting comparison of the independent work by the two groups [8] it is pointed out that Purcell and Bloch approached the problem in complementary but equivalent ways. Purcell saw it as resonance absorption of quanta corresponding to the energy difference between two quantum–mechanical states. For Bloch a classical picture stood in the foreground, the change in orientation of the proton magnetic moments*. (Brandt 2009, p. 294).

[28] *Chromatography proved to be a particularly important development. In its early period, the technique was used principally for separation but in time it proved adaptable to qualitative and even quantitative analysis. The introduction to vapour phase chromatography in the 1950´s made possible the rapid analysis of mixtures which had been analysed with greatest difficulty before* (Ihde 1984, p. 584).

chemical laboratories' tables. New equipment industries were created following the military logic of the standardization of the parts, which facilitated their consumption. A new sub-discipline appeared, instrumental chemistry (Morris 2002; Baird 2004). About this change in chemical laboratory procedures chemistry' historian C. Reinhard said:

> The end of structural determination by means of traditional chemical degradation and synthesis represented the core of the intellectual changes brought about in the 1950s and 1960s by the instrumental revolution… NMR became the main method for the fast and accurate acquisition of structural information, including evidence on the dynamics of molecules that had been unavailable before. With the help of these instruments, chemists began to unravel the three-dimensional structures, configurations, and conformations of molecules, work that had tremendous applications in both science and industry (Reinhardt 2006b, p. 209).

From the fourth chemical revolution, spin is incorporated into the daily practice of the chemical community[29] as evidenced by the research in synthetic chemistry of the American R. B. Woodward,[30] who took advantage of the arrival of new instruments such as nuclear magnetic resonance and insisted in the preparation of new, more complicated products, many of great biological and medicinal importance. The synthesis of morphine, cholesterol, cortisone, strychnine, penicillin and chlorophyll shared the onset of tranquilizers (such as Librium and Valium), as well as contraceptives.[31] The total synthesis of vitamin B12 is a milestone in the history of chemistry. The synthesis of this substance, with nine asymmetric carbon atoms, began in 1960 and required the participation of more than one hundred chemists from 19 countries working in two laboratories simultaneously (Zurich and Harvard) to conclude in 1972 when Woodward made the announcement, in New Delhi, at one of the IUPAC Conferences (Woodward 1972). To this must be added the way in which commercial macromolecules changed the way of "constituting" the world. The post-war period marks the beginning of the plastics era. The application of thermodynamics and chemical kinetics[32] to the systematic study of these materials was undertaken by different research groups, among which the one headed in Germany by H. Staudinger, Nobel Prize in chemistry in 1953.[33]

Molecular biology emerged prior to World War II by the integration of different disciplines[34] to answer a question that was a problem, how is genetic information transferred from one organism to another? The question was originally formulated by what was termed

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[29] For example after publishing an important research paper (Linnett 1961) in 1964 the British chemist J.W. Linnett published the book *The Electronic Structure of Molecules: A New Approach* in which he incorporated the spin in Lewis octet' model.

[30] Awarded with the Chemistry' Nobel Prize in 1965.

[31] Developed initially in Mexico by Rosenkranz, Djerassi and Miramontes (Hernández-Garcia et al. 2016).

[32] Free radicals initiate many polymerization reactions. In fact IUPAC has defined the chain polymerizations as those in which the kinetic carriers of the reaction are radical (with an unpaired electron).

[33] As Staudinger recalled on his autobiography: *Molecules as well as macromolecules can be compared to buildings which are built essentially from a few types of building stones…If only 12 or 100 units are available, then only small relatively primitive buildings can be constructed. With 10,000 or 100,000 building units an infinite variety of buildings can be made: apartment houses, factories, skyscrapers, palaces an so on.* (Quoted in Furukawa 2003, p. 235). K. Ziegler and G. Natta awarded another Nobel Prize to this field in 1963.

[34] Molecular biology was interdisciplinary by design 'a grand fusion of the methods, techniques and concepts of organic chemistry, polymer chemistry, biochemistry, physical chemistry, X-ray crystallography, genetics and bacteriology' (Furukawa 2003, p. 431).

the phage group (Mullins 1972).[35] However it is consolidated at the end of the contest with what the historian Kay have called the 'protein paradigm' (1993). Molecular biology displayed some features that can be summarized as: a stress in the unity of life rather than on its diversity 'it became far more convenient to study fundamental vital phenomena on their minimalist level, it means 'discover general physicochemical laws governing vital phenomena; macromolecules, specially proteins, became the 'principal focus' and the scale of interest was of the order of size of these objects and finally molecular biology depended upon the design, provision and maintenance of complex and expensive instruments (Agar 2012, pp. 254–255).

During the fourth revolution, computers were incorporated into chemical research practices and with them the programs that allowed "chemical calculations" since the incorporation of Extended-Hückel in 1963 by R. Hoffmann. In that same year began to work the QCPE (Quantum Chemistry Program Exchange) and 2 years later J. Pople introduces CNDO and W. Kohn density functionals. All of the above made chemists begin to think about the structure of matter in terms of quantum mechanics. They did so considering some of their principles but incorporating broadly empirical information from chemistry. Quantum chemistry appeared as a new sub-discipline of chemistry (Tsuneda 2014; Garritz 2014)[36] with new educational challenges (Chamizo and Garritz 2014).

L. Pauling promoted the idea that atoms make up molecules in his extraordinary book *The Nature of the Chemical Bond and the Structure of Molecules and Crystals: An Introduction to Modern Structural Chemistry* published at the beginning of World War II and in which he introduces the explanation of many of the properties of chemicals using quantum mechanics (Hager 1995). The quantum nature of atoms, as interpreted by physicists, allows us to understand the structure of molecules that make up and the molecular structure derives the properties of substances.[37] However from the fourth revolution and result of the work of the American theoretical chemist R. Mulliken (who won the Nobel Prize in Chemistry in 1966) this idea was changing. From quantum mechanics it has been described that an atomic orbital is a monoelectronic wave function that considers the attraction of the electron by the nucleus and integrates, in an average way, the repulsion of the other electrons. For Mulliken a molecular orbital is defined in the same way, except that instead of considering a nucleus several of them are taken.[38] Molecules are made up of atoms, which in turn are made up of nuclei and electrons. Molecular properties in turn explain the

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[35] Initially composed by M. Delbrük, A.D. Hershey and S. E. Luria who would get the Nobel Prize in Physiology in 1969 for their research on bacteriophage viruses. Years later other scientist from different fields were incorporated like Watson (biology), Tiselius and Pauling (chemistry) and Perutz (crystallography).

[36] As early as 1952 the British chemist Ch. Coulson published the highly influential book *Valence* which states that quantum chemistry is not an application of quantum mechanics to chemistry but a new sub-discipline of chemistry.

[37] How to explain molecular structure in terms of quantum mechanics is one of the main arguments of the reduction of chemistry to physics, which has been the subject of many studies, for example those carried out by Hendry (2012, 2013).

[38] *…the MO method, which in its most general form* ***regards each molecule as a self-sufficient unit and not as a mere composite of atoms….*** *In conclusion, I would like to emphasize strongly my belief that the era of computing chemists, when hundreds if not thousands of chemists will go to the computing machine instead of the laboratory for increasingly many facets of chemical information, is already at hand.* (Mulliken 1966).

characteristics of substances.[39] The molecule, and not the atom, appears as the fundamental specie of chemical substances as can be seen in Fig. 2[40] in which one of the contributions of the fifth revolution, supramolecular chemistry is advanced (Chamizo 2017a).

With the molecule as the fundamental chemical specie appeared, during the fourth revolution, a new situation very well characterized by J. Schummer:

> Nonetheless, there were two different kinds of species waiting for a decision on which should count as the basic one in chemical classification. The most important impact of spectroscopic methods was that it finally made chemists decide in favour of molecular species. Once established as independent means of structure determination, spectroscopic methods were also used to characterize quasi-molecular species for which there exist neither a corresponding chemical substance nor a classical approach of chemical structure elucidation, such as conformational states, intermediary states in solution, van-der-Waals complexes, molecular fragments in MS (Schummer 2002, p. 19).

With the incorporation of new instruments in chemical practices, the spatio-temporal approach to substances allowed us to recognize the complexity that this name alone … 'substance' encompassed.[41] The permanence of the elemental composition of a substance subject to repeated operations to eliminate its potential contaminants, the operational criterion that chemists use to distinguish substances from mixtures, no longer necessarily reflected the world that chemist approached. The old conception of substance, that traditionally did not consider time, could no longer be maintained (Bachelard 1973; Jensen 1998a, b, c; Needham 2010). Thus little by little the broader concept of chemical specie replaced the narrow one of chemical substance.

The current definition of chemical species in IUPAC's Gold Book indicates:

> An ensemble of chemically identical molecular entities that can explore the same set of molecular energy levels on the time scale of the experiment. The term is applied equally to a set of chemically identical atomic or molecular structural units in a solid array. For example, two conformational isomers may be interconverted sufficiently slowly to be detectable by separate NMR spectra and hence to be considered to be separate chemical species on a time scale governed by the radiofrequency of the spectrometer used… The wording of the definition given in the first paragraph is intended to embrace both cases such as graphite, sodium chloride or a surface oxide, where the basic structural units may not be capable of isolated existence, as well as those cases where they are. In common chemical usage generic and specific chemical names (such as radical or hydroxide ion) or chemical formulae refer either to a chemical species or to a molecular entity.

It is not a minor change. By replacing the concept of substance like that "stuff" found in a bottle, chemical practice imposed on the material world that surrounds us, just as with

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[39] *Atoms are nice, atoms are fundamental, but they're not chemistry. Chemistry is about molecules, the fixed but transformable way in which atoms get together for a while (Hoffman and Torrence* 1993*, p. 21).*

[40] After an initial proposal of Jensen (1998a).

[41] That, to say it briefly, seems more to what is meant by "stuff" (Ruthenburg and van Brakel 2008). The current definition of IUPAC's Gold Book of chemical substance indicates: Matter of constant composition best characterized by the entities (molecules, formula units, atoms) it is composed of. Physical properties such as density, refractive index, electric conductivity, melting point etc. characterize the chemical substance.

purity, the results of our experiments and the capacity of our instruments. With the displacement, without replacement, from substances to species the field of study of chemistry grows and becomes considerably complicated. The reaction mechanisms that were so successful in organic chemistry and that decomposed a reaction in a series of successive reactions considering the existence of several intermediaries could and were studied. Many of these intermediaries were nothing more than chemical species. Several of the most important instruments for its study are those that have to do with the spin, the entity of this revolution.

Finally, in 1965, the Chemical Abstracts Service introduced the CASRegistryNumber (CASRN) a computer system to identify any substance without requiring its name and since then the largest database related to their identity.[42] The compositional approach of the language of chemistry about substances, used since the first revolution, began to be replaced.

The fourth chemical revolution is not characterized by the resolution of a dispute, as was the case in the previous three but, after the massive introduction of instruments, significant changes in the emphasis of research and scientific practice and in the structure of academic and professional organizations were produced. It is an excellent example of Humphreys' emplacement revolution (Humphreys 2011, p. 132). The words 'plastic' and 'flexible' became commonplace and socially identified a valuable attitude, even though they also characterized, the first of them, the emerging world consumer society. Plastics were cheap, easy to produce everywhere and disposable (Bensaude-Vincent and Simon 2009; Bensaude-Vincent 2013; Meikle 1997). At the end of the fourth chemical revolution, with the new plastic fabrics produced by the increasingly powerful chemical industries, the artificial seems to dominate the natural. With the increasing presence of synthetic materials, chemists and their industry failed to integrate into the collective imagination what is evident and well known to them. A chemical substance is what it is, regardless of its origin.

From this moment physics and biology occupy a prominent place in the interest (molecular biology as a new sub-discipline) and thinking (quantum chemistry as a new subdiscipine) of chemists.[43] Spin appeared as a new 'stabilized' chemical entity.[44] The new

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[42] A CAS Registry Number is a unique numeric identifier assigned to a substance when it enters the CAS REGISTRY database. Numbers are assigned in sequential order to unique, new substances identified by CAS scientists for inclusion in the database. A CAS Registry Number is a numeric identifier that can contain up to 10 digits and has no chemical significance. The very broad concept of substance that CAS uses considers: Elements, Organic compounds, Inorganic compounds, Metals, Alloys, Minerals, Coordination compounds, Organometallics, Isotopes, Nuclear particles, Proteins and nucleic acids, Polymers, Nonstructurable materials (Unknown, Variable Composition, Biological). That is, not all are substances according to IUPAC, nor necessarily chemical entities. In June of 2017 CAS REGISTRY^{SM} contains more than 130 million substances. For an important discussion of this see: Ghibaudi and Cerruti (2017).

[43] This can be exemplified by Pauling: *I desire to solve the wave equation for simple organic crystals and molecules [and to] develop a set of atomic radii and of structural principles enabling one to predict with confidence the atomic arrangement, including interatomic distances, of the normal electronic states of any molecule, and its stability relative to other molecules. This knowledge may be of great importance to biochemistry, resulting in the determination of the structure of proteins, haemoglobin, and other complicated organic substances* (Quoted in Agar 2012, p. 248).

[44] Here it is important to remember Chang's approach to entities as was said above: *Historical epochs are marked out by epistemic objects (entities that we identify as constituent parts of reality).* Spin adds to the entities of the previous three revolutions appearing since then in chemistry textbooks. About the ontological autonomy of the chemical world where this characterization of "chemical" spin is located, Lombardi said: *When the ontologically pluralist perspective is applied to the relationship between chemistry and physics, a picture completely different from the traditional one appears. Once the epistemological irreducibility of chemistry to physics is admitted, the ontological priority of the physical world turns out to be a mere meta-*

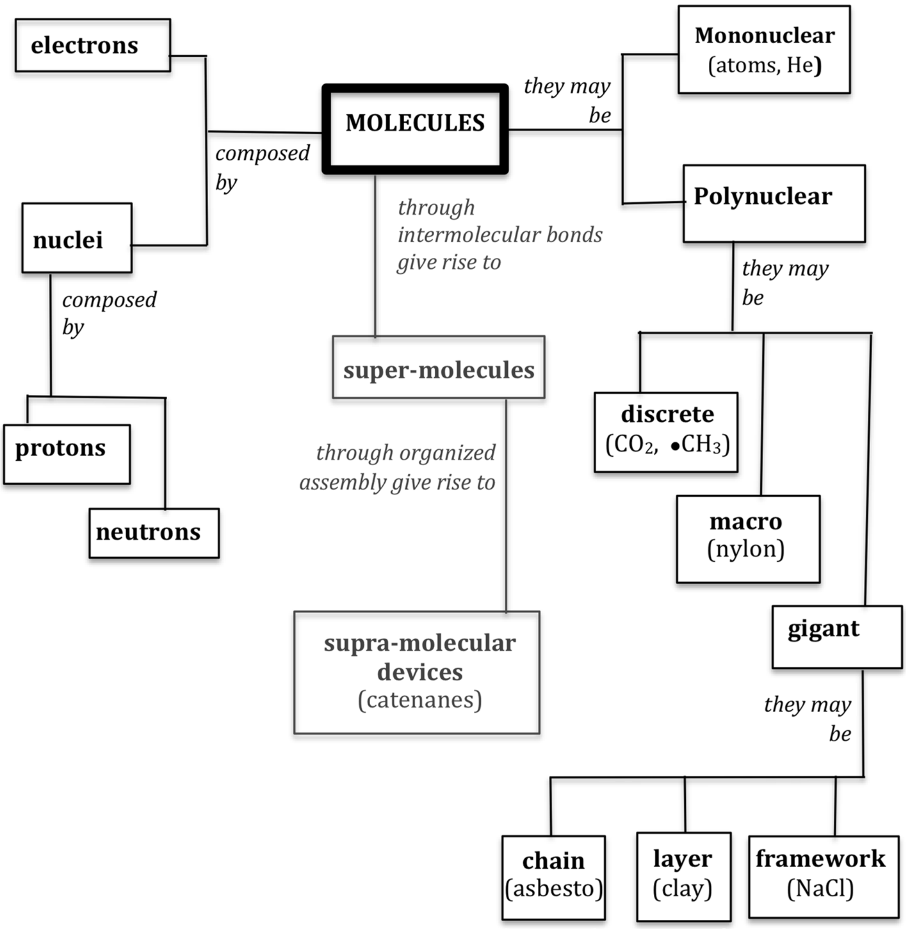

Fig. 2 Molecules, the central species of chemistry

exemplars that were part of the new textbooks written during and after this emplacement revolution indicated it.

Conclusions

> Making new worlds, as chemists have been doing for centuries, often depends on decomposition and composition (Goodman 1978, pp. 7–10).

Footnote 44 (continued)
physical prejudice. From the pluralist view point, concepts like bonding, molecular shape and orbital, refer to entities belonging to the chemical ontology, which only depends on the theory that constitutes it. Chemical entities do not owe their existence to an ontologically more fundamental level of reality, but to the fact that they are described by theories whose immense predictive and creative power cannot be ignored (Lombardi 2015, p. 23). See also Córdoba and Lombardi (2013).

With educational intentions five "long" Chemical Revolutions (or ruptures, discontinuities, transitions) mainly by emplacement procedures were identified through the incorporation of new textbook's exemplars, after being consolidated. A Chemical Revolution has been recognized by:

- A radical reinterpretation of existing thought recognized by contemporaries themselves, which means the appearance of new concepts and the arrival of new theories.
- The use of new instruments changed the way in which its practitioners looked and worked in the world. New entities were discovered or incorporated.
- The opening of new sub-disciplines, which produced, separated scientific communities.

During the Fourth Chemical Revolution chemistry grew and unfolded. Chemistry is not only inorganic, organic or physical, but also with the incorporation of new instruments, deeply analytical. On the other hand, the irruption of computers and different spectroscopies, with its multitude of instruments, forced chemists to learn the language of quantum mechanics which gave rise to another sub-discipline: quantum chemistry. From this moment, the name of substances, coined after many years of social conventions, began to lose its status as a reference of identity. Thus many chemical communities surpassed substances to work with chemical species: the set of stabilized identical chemical molecular entities.

As Gyung Kim said:

> Chemist acquired the power to make and re-make their worlds much earlier than other scientific practitioners…Their remarkable success in stabilizing and universalizing their laboratory reality depend critically on their dogged pursuit and promotion of the analytic-synthetic ideal of chemical substances…(Gyung Kim 2014, p. 118).

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