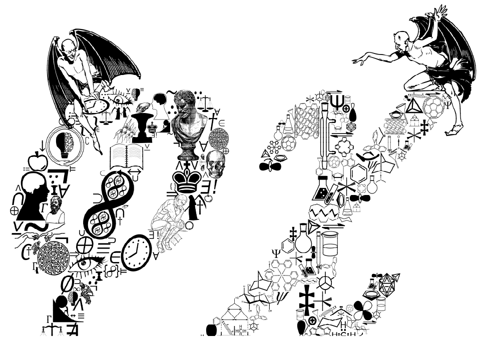
How Scientific is Chemistry?

Sebastian Kozuch

Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva 841051, Israel. kozuch@bgu.ac.il

To my father, who loves philosophy and science, but is not really engaged into philosophy of science.



Abstract

φ for philosophy, χ for chemistry. Is there a connection? Is there any interaction? Do chemists have something useful to learn from philosophers? Do philosophers from chemists? How can we define if chemistry is a science, or at least trustworthy? Which disciplines, styles and personalities are progressive in chemistry? Which ones are truth-seekers, progress-seekers or profit-seekers? Is there a point in asking these questions? Is there even an answer to them?

Introduction

Yes, of course chemistry is a science. That is beyond the point. The question is not if it is a science, but how good a science is it. Or, as we can put it, what is the *scientificity* level of chemistry, a term defined as the degree or quality of the discipline or project (compare to "viscosity", "luminosity" or "exergonicity"). To be clear, in some sense chemistry might even be considered the top science: It does not confront the complete unknown solely with statistical analysis, such as in many areas of life sciences, and it does not participate in purely esoterical mathematics, such as in some areas of theoretical physics. However, there are other scientific measures that chemistry does not completely fulfil, like its incapacity to achieve complete reductionism (more on this later on). Importantly, do not confuse "scientificity", a quality, with "scientism", usually taken as the critique to the arrogance of science (especially to hard, western, white, male, patriarchal, and capitalist science).

So, what is this article is about? It is a rudimentary, eclectic and partial trip to the land of philosophy of science. It is a subjective evaluation of the status of chemistry as a science. It is also an exercise on understanding the limits of good science.

As a note, while being outside the frontiers of science might sound dreadful for chemistry geeks, let us not forget that many openly non-scientific disciplines are completely valid. Modern-day alchemy, all kinds of alternative healing or new-age environmentalism indeed are the pseudoscientific ghosts that haunt us, contributing to a general feeling of chemophobia. No nice words will be spent on that here. However, engineering, scientific communication in all of its forms, or, in line with this article, philosophy and history of chemistry, are examples of non-scientific disciplines that can perfectly be progressive and insightful.

Many of the things to be discussed here are quite obvious for a chemist, and many are quite obvious for a philosopher. Since clearly having a *philosophiae doctor* title does not make me a philosopher, I acknowledge that many of the philosophical terms that I am using are taken in a colloquial, imprecise or maybe even slightly erroneous way. The profuse discussions on the correct definitions of such lexicon (or the confusions created by the many meanings of philosophical terms) can be found in the not so popular (yet) philosophy of science literature. Furthermore, being a non-strictly scientific opinion piece, I took the liberty of composing it in a light tone, with more interest in presenting an overall idea and having an amusing reading than in seeking for accuracy or completeness (this is for you, reviewer two![1]). In doing so, and slightly in the style of some renaissance discussion books, I will introduce two characters that will aid in the depiction of concepts and viewpoints: Tris the Chemist, and her workmate, Kris the Chemist. Tris and Kris will act as different persons on each section, always contradicting the other, always showing a different style of chemists, always believing their way is the best way (any similarity to actual persons is purely coincidental; or maybe not). I will ask here for the reader's forgiveness on the matter of shortage of references, definitions, precision and seriousness when trying to make a point on how scientific chemistry is. For more information, see for instance refs. [2–4], from where most of the material of this article was taken.

On the Nature of Induction and the Demarcation Problem, or How to be a Fundamentalist and Ruin the Scientific Party

Kris the spectroscopist tells Tris that the recently obtained rotational spectra of the Eagle Nebulae shows the presence of cordrazine, proving his hypothesis about the synthesis of complex organic molecules in interstellar dust. Tris the pedantic chemist, a proper Popperian, vehemently disagrees, arguing that this observation does not epistemologically prove anything, as it is always possible that the cordrazine came from a different source, for example from space alien's droppings. For Tris, only proving the lack of cordrazine would have some meaning, that is, it would falsify Kris' hypothesis. Kris groaned. This story has a very sad ending in terms of friendship between these two fellow chemists.

This discussion between Tris and Kris is possibly at the heart of the demarcation problem and the fight between what is called "the problem of induction" and progressiveness.

Karl Popper was, for better or worse, the personification of *the* big question in philosophy of science. He had an obsession: to delineate the boundary between science and, well, not-science. For that, he developed the idea of *falsifiability*,[5] which can be said to be the epitome of scientific honesty, but it is also a dangerous and impossible idea. While accepting failure is part of everyday science, Popper went on to say, almost fanatically, that there is no empirical confirmation of anything, only refutation. If you have a hypothesis, it must predict something; if the prediction is correct, good for you, but it does not prove that the hypothesis was confirmed; if the prediction is falsified, then we can be sure that you are a looser.

Induction is the "proving" of a hypothesis by the observation of N facts, while its (relatively obvious) problem is the impossibility of being absolutely sure, and the difficulty of logically justifying the hypothesis by those facts, even with $N \to \infty$. This was famously pointed out by David Hume, and commonly exemplified by the black swan example (the "All swans are white" statement was an evident fact until it was falsified by the description of beautiful Australian black swans in 1790). As Popper claimed, there are no "confirmations", only "corroborations" (you must embrace semantics if you want to do philosophy).

Progressiveness in science involves the discovery of new laws, effects and entities, and the production of novel advances. Lakatos is the name to look for when starting to learn this concept. According to him, a *scientific program* is progressive if each new theory or model construct something empirically new based on the previous model, with the power to predict, and obviously these predictions are proven to be true. If not, it is a degenerate scientific program. As everyone else in philosophy, Lakatos was heavily criticized, since fighting seems to be the philosophers' way. Still, his formulation of scientific programs made a profound dent in the philosophy of science. But I am digressing.

Science should be completely honest and accurate, which is an impossibility if we employ the "almost" honest inductive method. At the same time, science has to advance, an impossibility without generalizing observations, that is, making inductions. We cannot have both. To progress we must err, but to achieve infallibility we must test our hypothesis *ad infinitum*. What can a high scientificity discipline do with this paradox of failing to be both progressive and wholly scientifically honest? It can do its best; walk through the tightrope between these two competing conceptions of scientificity, or as Voltaire poetically articulated: "*le mieux est l'ennemi du bien*" (the best is the enemy of the good). As we shall see, these scientificity paradoxes are omnipresent.

Regarding chemistry, it is my belief that we are fine. In experimental chemistry we do need many measurements to achieve certainty beyond any reasonable doubt on every data point, which makes us prone to some residual uncertainty. However, Hume's problem is minimized by the high reproducibility of chemical systems. How many times do we need to measure the melting point of vanadium to include the number in thermochemical tables, without the fear that one day it will be falsified and melt at 100 K lower temperature? Luckily for us atoms are atoms, not rats.

Sometimes we must be extremely careful on measuring due to the sensitivity of observable effects (think for instance about the exponential relationship between energies and equilibrium constants). But once in a blue moon this exponential sensitivity let us reach an epiphany, for instance when finally finding the right conditions for the high yield synthesis of cordrazine after running a shedload of experiments. Sometimes it is actually the opposite, when instead of seeking a particular chemical objective we just mix many reactives and check what product might be obtained[6] (a part of what we call "serendipity").

Still, beyond some uncertainties kindly brought by Heisenberg, molecules do not have tantrums. This chemical accuracy usually (but not always) gives a thick layer of validity to inductive techniques in chemistry. As such, honest chemists are less worried about falsifiability, since high reproducibility is not a fantasy in our field (and I repeat, we speak of honest chemists). In addition, as argued by Roald Hoffmann: "*Falsifiability works well for establishing reaction mechanisms, but has very little to do with organic or inorganic synthesis. When a molecule is made, or modified, falsifiability is irrelevant. Chemistry is much about creation as about discovery*".[7] In essence, the problem of induction and Popperian's extreme falsifiability viewpoint are hardly chemical problems.

If you are still looking for arguments against induction, I do recommend to try to understand Goodman's mind-blowing "grue" riddle.[3]

On the Nature of "The" Method, or How to Destroy a Childhood Fantasy

Kris and Tris are very good friends in the chemistry department. As such, they enjoy gauging each other's eyes whenever they can. Kris made a reputable career establishing thermodynamic tables of thousands of compounds with a marvelous accuracy. Tris is a maverick physical chemist, trying to define when (and not if) the parity violation of weak forces produces an observable and significant difference in enantioselective autocatalysis, an incredibly difficult task. Kris tells Tris that she will never receive tenure if she will not start publishing seriously, while Tris answers to Kris that he will never publish a Nature/Science article, and for sure he will never get a Nobel. Kris is very sad, since he thinks that Tris is not doing real science. Tris is also very sad, since she thinks that Kris is not doing real science. So they bury their mutual sadness together, sharing many beers.

We saw one condition for the demarcation of science in the keen and elegant proposal of Popper's falsifiability. And we also saw that it is more a holy grail than a down-to-earth scientific reality, if we take it to its extreme. The reality is that on the matter of what produces high scientificity research everybody has an opinion, nobody has an answer, and everyone thinks that the opinion of others stinks. But there is still a large consensus on many conditions that demarcate science, small consensus on others, and an additional consensus saying that no answer is definitive. In addition, many conditions contradict others, as we saw above and will see below. Nevertheless, we can briefly discuss some of the most basic rules that lead to high scientificity.

First of all, we must agree that the *scientific method* does not exist. It is a myth. Don't you believe me? Try to define it in very precise terms, beyond the idle "postulate hypothesis – do experiment – prove hypothesis" high-school characterization. You cannot. For the same reason that nobody else could. Laboratories cannot and do not practice science under the same set of rules, as exemplified by Kris and Tris. Which brings an interesting dichotomy: shall philosophy of science be *normative*, and tell scientists how to work, or should it be *descriptive*, and just observe and analyse how scientist work (or as it was explained, "like ornithology to birds")? We will not answer this question, but just for you to know, we are being observed.

Nonetheless, even if we lack a definitive scientific method, nobody doubt that its spirit is an intrinsic part of us, and without it we might fall to the dark side. We all practice the main scientific activities of studying, hypothesizing, testing, observing, analysing, deducing, and/or concluding, not necessarily in that order, and many times looping between them. For instance (and I am making up a possible chemical project), you expect to design a metal-organic framework that would work as an electrode for CO_2 reduction. You study the literature, hypothesize that this particular ligand with this particular metal might do the trick of letting the electrons hop, you create the MOF, characterize it and measure some electrochemical curves, and obviously conclude that nothing works, as always. So you restart the process over and over again, until it miraculously works (at least partially), or you find by chance some other interesting effect, or it does not work at all and you try a somewhat different path. Is this a method? Yes, to a certain degree, and no, since what you really did was flowing with the project's vicissitudes, adversities, frustrations and eurekas.

And yet, the fact that we are (or we aspire to be) true to the experimental results, open to new observations, sincere with negative values, and rooted on strongly based theories and models distinguishes a scientist from a non-scientist. Most of chemistry is fine with this, whether we call it a method or not.

On the Nature of Deduction, or How to Trust Yourself When you are Definitely Wrong

Kris, a graduate student, goes to Tris, his supervisor, and asks her how she can explain these NMR peaks obtained after the synthesis. Tris explains with the patience that every PI has with their students: "It's easy, with the dioxirane in a coarctate reaction you obtained an epoxide, exactly as the theory says about pericyclic reactions". A day after that, Kris rushes to Tris office and tells her that the spectra got mixed, and the actual peaks look very different, to what Tris answers: "Then it's easier! with the dioxirane and the sulfidic substituent you obtained sulfoxides, exactly as the theory says".

The *deductive method*, the nemesis of induction, consist in the use of logical inferences to obtain conclusions from statements, without the need of unsettled and unsettling inductive generalizations. It is the highest epistemological way of obtaining sound conclusions, and as such, it is very problematic. If the deductions indeed are completely "kosher" (which is not always the case), who says that the statements (usually experimental observations) are truthful and complete, as Kris just found? Let us not fool ourselves, this flash-fiction of Kris and Tris is way more common than what we dare to admit, and these logical acrobatics that we use to fix our faulty rationality are a sign of low scientificity. To err is human, and to sweep it under the rug is more so. Scientists are humans (believe it or not), but science is not.

But beyond these dinosaurian size technicalities, chemistry is well based in deductive reasoning only when we distinguish the difference between theory, law and model. In unsophisticated and imprecise terms, a theory is big and as close to the truth as we can have. A law is small but also quite faithful to reality. A model is different: it works, until it does not work anymore. "Quantum" is a theory; "Le Chatelier's" operates as a law (even if it is commonly known as a principle); "octet" is a model, a superb one, but it only works when it works (i.e. with main group, non-radical and non-bizarre chemistry). *Knowing a model means knowing its limits*. Whoever tries to stretch, for instance, the VSEPR model to fit the data of the nonconforming disilene geometry should receive a slap on the wrist for not adhering to the model's limits. However, deductive explanations of disililene geometry by quantum mechanics or by the Jahn-Teller effect (a more precise model), is a high scientificity deed. Bear in mind that even theories have limits, and therefore they can sometimes be taken as models (like Schrödinger missing relativity), but let us not be so pedantic with these definitions now.

In the superior cycles of philosophy of science it is argued that even the purest deductive reflections are faulty. Kuhn in his celebrated[8] (or notorious[9]) book "The structure of scientific revolutions" postulated that we live in a paradigm, which tells us what to see and what to ask, but that one day a revolution will produce the paradigm shift that may even change the questions and how we see reality (libraries were written on this idea, so we just describe the tip of the tip of the iceberg). For Kuhn, only Lavoisier produced a big enough change to deserve to be called "the" chemistry revolution; but micro-revolutions are there in front of us popping up from time to time: DNA structure, DFT, Fukui's frontier orbital theory, STM, etc. With such discoveries shaking our ground, how can we trust our deductions? Our observations themselves are *theory-ladened*, as philosophers like to call it. Moreover, according to the Duhem-Quine thesis any test of a scientific hypothesis will be inconclusive no matter how good our deductive powers are; background assumptions, alternative explanations, ad-hoc hypothesis, and so on (the "Münchhausen trilemma" is an interesting entry point to the topic).

To put it in simple chemical words, if you do not like your product, you are free to blame the omnipresent traces of water, the approximations of the model, the lousy sensitivity of the NMR in your chemistry department, or many more imaginative solutions that can solve the guilt of your failure. In philosophical terms, these explanations are still logical assumptions. I am not advocating for such justifications, but everybody knows that the outcome of our extremely sensitive analysis can be affected by the colour of our socks, right? Enough imagination and flexible ethics can take us a long way (albeit many times into the dark side).

So we must, again, walk through the tightrope. There is an equilibrium between being faithful to our observations, and making *ad hoc* assumptions to "fix" the observations and keep our deductions in check. The rules to decide if our justifications and excuses are valid or not are not written in stone, and whatever is high scientificity for one chemist may not be for another one. For one researcher an annoying experimental datapoint might be an outlier that can be safely neglected; for another researcher that point can significantly change the average melting point of Vanadium. Only one of them is right. Again, it is hard to be fully scientifically honest and progressive at the same time, when we have place for subjectivity.

On the Nature of Scientific Explanations, or How you Can Live With or Without them

Tris has a method: mix, heat, characterize, publish. Kris also has a method: hypothesize, mix, heat, flash, test, change, add, observe, hypothesize, mix, heat, spectra, XRD, DFT, TEM, TLC, NMR, AFS, propose mechanism, one more test to be sure, and publish. Tris makes fun of the perseverance and naivety of Kris' perfectionism. Kris thinks that Tris is great as an engineer, not a chemist. Both of them are very proud of themselves and their "true science".

Some thinkers take it very simple. If it works, it is science. For some others, if it explains, it is science. And for the most pragmatists, if it can be published, it is science. Even if these are simple and almost childish ideas, we must never underestimate the philosophers' power to convolute simple ideas.

Explaining has been, almost poetically, defined by Duhem as "*To explain… is to strip reality of the appearances covering it like a veil, in order to see the bare reality itself*". For the Latin lovers (I mean the Latin language enthusiasts, not the stereotyped Hispanic seducers), we have two new terms that are usually found in philosophical texts: *explanandum* is the phenomenon that has to be explained, and *explanans* are the statements that explain the phenomenon. Interestingly, some philosophers do not like to ask "why" the explanans explains the explanandum in science, since it involves intention; they prefer to ask "how", since explaining is just describing observations based on established scientific laws. I fail to distinguish if this is a serious semantic issue, of if it is a matter of tomato, tomahto. Nevertheless, as my postdoc advisor use to say, "my favourite question is *why*".

In the Tris and Kris fable, Kris is very fond of trying to strip the veil of his experiments and seeing, if accessible, the complete reality of the mechanism of his reaction. For him not understanding the "arrow pushing", the electronic density and the determining states of the catalytic cycle is unconceivable, since science is understanding. And without understanding there is no prediction, and without predictions there is no science. It is a valid point that most chemists agree. Just not all of them.

Tris does not care much about explanations. She is a fan of discovering, not of explaining. Explaining might come in the future by people like Kris. Many might consider Tris' approach as "dirty science" or "stamp collecting" (quoting Rutherford's attributed statement: "All science is either physics or stamp collecting"). However, let any one of you who is without sin be the first to throw a stone at her. Most fads in chemistry started as educated versions of "let's mix and see": nanochemistry, organometallic complexes, drug discovery, etc.

Even in theoretical/computational chemistry, while surfing through equations and high-performance computing, many times we throw the towel and say "just run all the scannings, one of them will get us a lower transition state". Or we say: "look at this, neglecting these coupled cluster terms actually got us better accuracy in multireference systems, who could have guessed that?". These *in silico* discoveries are valid science, even if they are absent of explanations. As in Tris' style, in theoretical chemistry it is also valid to leave the explanations to the future (although less common compared to experimental chemistry).

Thus we have the explanationists and the "stamp collectors" as prototypical scientists. We really like explanations like Kris, but we are also disciples of Tris here, and in the 21st century no scientist cosplaying as a philosopher will speak less of this approach as long as it is done in a scientific way. A good scientist acknowledges serendipity, the mix and see approach, and the beauty of the surprise discovery. We created whole scientific fields to exploit this: combinatorial chemistry, machine learning, molecular docking, etc. High scientificity "stamp collecting" research is the one that, based on accurate models, can correctly find the molecular needle in the database haystack. This is common scientific knowledge and part of the mythical scientific method. We do not really need to be philosophers to recognize this.

Among philosophers of science there are explanationists, as seen above, and predictionists, who say that science should be more about generating novel and correct predictions than about explaining old observations. Between them, we have the accomodationists (I swear I am not making up these names) and the formalists, both of them accepting explanations and predictions as signatures of high scientificity, but putting a different weight on each one. Chemistry has been very successful in explaining, especially since the paradigm of the existence of atoms and the chemical bonds has been validated over and over (in these days we can even "see" atoms and their electronic densities thanks to AFM, STM and other techniques, plus quantum computational chemistry if I may stretch the meaning of "seeing"). However, chemical predictions are another story. Most hypothesis are small predictions that can be, ideally, tested experimentally, and as we all know, most experiments go wrong.

It has been said that the difference between science and art is that in science we accept the experimental failures, while in art we just call them "experimental art" and put them in the Centre Pompidou. Beyond this unfunny joke we can extract a simple and controversial scientificity opinion: if it works, it is science. This is not as extreme as it sound, since our scientific method, if it exist, involves making use of the trash can if our hypothesis turns out to be incorrect; but if it provides a correct prediction, then it is progressive.

Is chemistry scientific in this sense? Very. Chemistry has accessible facilities to answer most of our predictions, especially compared to other disciplines that sometimes require fortunes to test theirs (think of the dimensions of the equipment to prove the existence of Higgs' boson). We also have, usually, much less conflicts of interests than other fields, and a much stronger base of laws and theories to root our hypothesis compared to others. In summary, we have, arguably, good enough means to explain and to predict (or at least to falsify our predictions).

And then, of course, beyond explaining and predicting we have the "publish or perish" measure of scientificity. This should not be overlooked as a ludicrous ambition of megalomaniac researchers; we are, at the end of the day, the sum of the impact of our research. We just need to keep a leash on our narcissism by remembering Goodhart's law: "When a measure becomes a target, it ceases to be a good measure". In any case, this is not a matter of philosophy of science, but of sociology of science, and therefore this publishing discussion will be mostly left out of this article. If this is relevant to you, be content that chemistry publishes more and faster than other disciplines.

On the Nature of the Ivory Tower, or How Hydroxyapatite Moves the World

Kris has established himself in the R&D section of a large agrochemical company. His work consists in developing a cheaper, more efficient and greener large-scale method for the production of pyrethroids. In the opposite corner, Tris has established herself in the organic department of a large university. Her work consists in developing a cheaper, more efficient and greener small-scale method for the production of pyrethroids. Tris thinks that Kris is a great and brilliant guy, just not a scientist. Kris thinks that Tris is a great and brilliant gal, just a bit snobbish; and that she should keep her opinion in her pocket (to put it politely).

"Science is what scientist do". As foolish as it may sound, this statement is quite close to the truth. The focus of academic science is more knowledge-directed and less objective-directed than "industrial" science; the infrastructure of research institutes is made for science; there is openness to research sharing; the publishing system, as imperfect as it is, provides filters to avoid the proliferation of pseudosciences. In summary, scientists do science in the scientific system.

Philosophers seem to be divided on this. Nobody dares to say that universities have a scientific monopoly. However, some thinkers consider science as a social enterprise that is achieved by internal debates in a scientific society. Popper, the logical positivists (browse the "Vienna Circle" to learn about them) and others were obsessed in trying to define the limits of science, struggling to define what is reality and truth, or debating what can and cannot be observed in an experiment. This approach is universal, and their philosophical conclusions can be applied to university-style science, industry-style science, or even to movie-style lone-wolf scientists (who usually want to conquer the world, of course).

On the other side, people like Kuhn and Lakatos focused more on scientists fighting and interacting, the structures they build, and how the society of science deals with real life science. All the disputes about the role of paradigms and revolutions (Kuhn's pet model) and research programs (Lakatos' idea) involve a community, which must be centralized in an ivory tower.

In awfully simplistic terms, a paradigm is, as said above, the big foundation where a discipline stands on, and therefore taking it out means having to restructure the whole field. For instance, in chemistry we have the humongous paradigm of the existence of atoms, molecules and bonds; it is unthinkable to consider it as just a hypothesis. But buildings were destroyed in the past when enough experimental weight accumulated, such as with the demolition of phlogiston theory.

Lakatos' research program came to fix some deficiencies of Kuhn's model, and involves a "hard core" theory with a "protective belt" of auxiliary hypotheses, since in reality no theory is exempt of difficulties which should not make wrecking theories a daily matter. For example, the discovery of quasicrystals does not mean that all the crystallography textbooks must be rewritten.

Many other philosophers were involved in such surprisingly bloody debates on the sociological and psychological aspects of science, including Laudan, McMullin, or even Feyerabend, who we will meet later on. But only Imre Lakatos had a life deserving a Hollywood film (possibly directed by Christopher Nolan and with Leonardo DiCaprio, just an idea). I do recommend reading about his adventures. But I am digressing again. The point is that to have a debate about what is and what is not part of a field, its basis and scope, we need a unified, integrated community.

What about chemistry? Well, chemistry is what chemists do. Sure there are anecdotes of discoveries made by individuals outside the club, with the Mpemba effect as a superb example (a Tanzanian schoolboy discovered that under certain conditions hot water freezes faster than cold water, believe it or not). But except for these black swans, all the "simple" chemistry was already done a long time ago, and new discoveries require the infrastructure (equipment, libraries, networking) that only a research institute can provide.

Right now, August 2020, there are some "citizen scientists" testing do-it-yourself nasal Covid-19 vaccines made from available epitope peptides. The answer from the establishment is that the multi-billion budget from the public-private partnerships in two hundred vaccine research projects done in top universities and multinational pharmaceutical companies would probably have already found the vaccine if it was that easy. Citizen-science still has many advantages in terms of being extremely educational and a fine hobby, while it might even aid in a few discoveries (several examples in amateur astronomy, zoology and botany). A chemical exemplar is the "solar army" of high school chemists recruited to check the gazillion different combinations of possible semiconductors that may be used to photochemically split water.[10] Nonetheless, whatever would be discovered by this students army, it will be tabulated and published by the academic big brother.

We must not rush and exclude industrial and private chemistry labs from the "high scientificity" label, even if they live in the "patent, not paper" culture. This is not only on account of the output of monumental international high-tech, pharmaceutical or petrochemical companies, but also due to the myriad of chemical start-ups that are transforming the face of chemical R&D. Moreover, the industry, although much more conservative than the academy, is less forgiving regarding the lack of results. If the new synthetical method for pyrethroids is not really cheaper, greener and more efficient, Kris might be invited by his company to find another job, while Tris can still be saved by her university tenure. The "scientific honesty" of academics is not the only way (and sometimes it is not the way) to avoid the epistemic viciousness[11] that may grow in the academy if unchecked.

But for sure we cannot leave to "Google university researchers" to define chemistry or we will be doomed, as happened with the dihydrogen monoxide shameful panic hoax.

On the Nature of Reductio ad Absurdum and Creatio ex Nihilo, or How Barba non Facit Philosophum

Tris is a hardcore physical chemist who believes that Schrödinger's equation has "the answer to the ultimate question of life, the universe, and everything". Kris is a biochemist. Enough said.

One of the most interesting debates in philosophy of chemistry (yes, we do have our own philosophy branch[12–19]) is the discussion about reductionism and emergence. That is understandable, considering that we are the ham of the scientific sandwich, between physics and biology (some people argue that the ham is the most proteinaceous part, just saying…).

Reductionism implies the study and comprehension of large systems by understanding its small components and their laws (as all the other definitions in this article, it is a lousy definition; for the real stuff start with Nagel's *et al.*,[2] or Scerri's work making a case for chemistry[14]). You can, in principle, reduce genetics into molecular biology, classical thermodynamics into statistical mechanics, or the whole chemistry world into $\hat{H}\Psi = i\hbar\partial\Psi/\partial t$ [20] (plus some corrections, to be exact[21]). The connections between the reduced and the reducing theories are sometimes called bridge laws. Both reducing and finding the bridge laws is considered a high scientificity achievement, and often reduction is taken as a synonym of explanation.

The reducing field is sometimes considered to include in it the reduced field, and to be closer to the universal truth (whatever that might be). Since the catchphrase says that chemistry is reduced to physics, physicists love reduction; chemists, in contrast, have a justified trauma and inferiority complex with it.[14,22] However, philosophers and good scientists are very careful not to make a value judgement from this; reduction is a highly valuable scientific tool, but hardly the only one. In any case, if we want to feel better, we can always say that biology can be reduced to chemistry!

Life scientists love emergence. *Emergence* might be defined by the development of properties in a system, properties that its own small components do not possess. Bulk water is not molecular water, a metal-organic framework is not metals in an organic framework, adamantane is not protons, nucleons, electrons and a wave function to rule them all, and life is not fats, proteins and sugars adorned with nucleotides. Biology can be considered semi-metaphorically as an emergent property of chemistry, as much as chemistry is an emergent property of physics. Finding emergence is considered a high scientificity achievement, and for some people even a higher feat than reducing.

The curious thing is that trying to achieve high scientificity through both reduction and emergence is contradictory. The former is connected to order and deduction, the latter with induction and chaos. It is possible to find water's triple point from reduction to quantum chemistry, but to do that you must model computationally a very large number of molecules (or more accurately an infinite number of molecules using the periodic boundary condition trick). In doing so, you are creating/discovering/observing new laws that were intangible by scrutinizing the reduced model of one molecule, even if hypothetically all the information was already there. Emergence can therefore be obtained from reduction, but only at the regime where reduction is completely loss, another paradoxical relationship. Hence chemistry is chemistry, not the pubescent offspring of physics (and for the arrogant chemist, please stop undervaluing biology). In the end, there are many ways to achieve high scientificity, but it is impossible to use all of them at the same time.

A fairly debated attribute of scientific explanations is the fact that they are generally one sided, always going from the explanans to the explanandum, as in:

- Pauli repulsion ⇒ steric hindrance in adamantane.
- Central dogma of molecular biology ⇒ methylation decreases MCT3 protein expression.
- Franck–Condon principle ⇒ fluorescence.

Similarly, reduction and emergence are one-way roads. Moreover, the number of explanans and reducing laws is always much smaller than the number of possible explanandums and emerging properties that can be observed in the lab. A direct analogy can be found in the second law of thermodynamics and the entropic timeline: going back in time we go to a lower entropy structure, equivalent to finding the explanans and reducing science to its more "ordered" laws; going forward we might find complex far from equilibrium dissipative systems in steady state, analogous to discovering emergence. This seems to me a fascinating topic, but *barba non facit philosophum*, so I will leave this discussion here.

On the Nature of Science and Pseudoscience, or How to Reach Science Fiction

Tris: Why have you forsaken me?
Kris: You have lost your way, my child.
Tris: Have not you say that the path of the righteous lies where the path has not been laid?
Kris: I did.
Tris: And yet I laid my path, as a stranger in a strange land, following your doctrine and preaching.
Kris: You did.
Tris: Behold me now, I am a leper kneeling before you, asking to be cleansed.
Kris: You are.
Tris: Then why have you forsaken my wicked soul?
Kris: Because you are researching cold fusion.

Where shall one start if trying to draw the demarcation line? Philosophers have tried for more than a century with large success in term of ideas, some of them very obvious, some of them quite ingenious, but with little success in terms of closing the matter. One problem is that the typical approach to draw the line is by deciding *a priori* which disciplines are science (chemistry, astronomy, immunology, etc.) and which are not (alchemy, astrology, homeopathy), and then trying to define the similarity and dissimilarity rules; however, the direction should be inverted, first the rules must be sealed, and the fields must be split up *a posteriori*. Many philosophers abandoned this quest, saying that finding the necessary and sufficient conditions to separate science from pseudoscience (or non-science) is like tilting at windmills.[23] Not only strict rules for science à la Popper fail to include many sciences, and soft rules like the "explanatory power" fail to eliminate some pseudosciences, but also there is a grey area where proper science can fall and (much more rare) pseudoscience can rise, given enough time and evidence ("there is no such thing as quasicrystals, only quasi-scientists" said Pauling three decades before Shechtman got Nobeled). Feyerabend, the big anarchist of philosophy of sciences, sharply ended his "against method" book saying:[24]

"…wherever we look, whatever examples we consider, we see that the principles of critical rationalism… and the principles of logical empiricism… give an inadequate account of the past development of science as a whole and are liable to hinder it in the future. They give an inadequate account of science because science is much more 'sloppy' and 'irrational' than its methodological image. And they are liable to hinder it because the attempt to make science more 'rational' and more precise is bound to wipe it out… For what appears as 'sloppiness', 'chaos' or 'opportunism' when compared with such laws has a most important function in the development of those very theories which we today regard as essential parts of our knowledge of nature. These 'deviations', these 'errors', are preconditions of progress… Without 'chaos', no knowledge. Without a frequent dismissal of reason, no progress…"

The "everything goes" philosophy of Feyerabend, as it is commonly known, has more detractors than friends, although it makes a point that nobody ignores. But make no mistake: even the harshest opponents of a stringent demarcation make it very clear that distinguishing science and non-science is critical for the sake of humanity. There are undeniable traits that are characteristic of science (even if they are not necessary and sufficient), and traits that are not part of our scientific world. However, to reach a consensus on which traits are in or out is, again, tilting at windmills.

We saw falsifiability, deductivism and inductivism, a scientific method, a centralized power, empiricism, reduction and emergence, progressiveness, research programs… what else do we have in the toolbox to define science?

- Kuhn spoke about a set of epistemic values: accuracy, consistency, scope, simplicity and fruitfulness.
- Judge Overton's opinion in the case about teaching creationism in class (McLean v. Arkansas Board of Education, 1981) was that science must be guided by natural laws, be explanatory with reference to natural laws, testable empirically, with tentative conclusions (i.e. fallible and autoregulatory), and falsifiable.
- Thagard, who dealt more with what science is not and less with what science is, adds the concept of "correlation thinking" in science against "resemblance thinking" in pseudosciences (an example of resemblance thinking is the "like cures like" homeopathy doctrine); he believed that pseudoscientists were oblivious to alternative theories and progressiveness.
- Mertonian norms, doing more sociology than philosophy, say that some scientific signatures are communism, universalism, disinterestedness, and organized scepticism.
- Other terms that usually appear are relevancy, insightfulness, substantiality, reproducibility, robustness, novelty, autoregulation, coherency, and so forth. Digging more it is possible to find a large number of philosophers giving many more new and refurbished ideas. Basically, where you have two philosophers there are three opinions (old Jewish joke).

Going back to chemistry, we can feel proud to say that there is practically no scientificity box that is left unchecked (except for full-throttle Popperian falsifiability, which as we saw it is actually a fantasy). But in specific lab projects it is practically and theoretically impossible to reach high scientificity with all these parameters at the same time. As said above, complete falsifiability and complete progressiveness are incompatible, as well as finding reduction and emergence, or trying to predict new effects and exploit serendipity.

We can also work by doing baby steps with high certainty of small success (like making small substitution in the catalyst second sphere to tune the reaction rate), or by making risky steps that might led to a breakthrough (like testing a completely new family of complexes when the previous family reached its maximum efficiency). The "high risk – high gain" approach works to some extent according to Feyerabend's anything goes position, or in some measure under Sturgeon's law ("90% of everything is crap"), with the hope that from ten grant-supported projects at least one will be objectively successful in the long run. Working under both styles (baby steps and risky steps) is like playing the two cards of Kuhn's model: help the progress of normal science, but at the same time open a door for a revolution. Both certainty and risk can produce high scientificity, but as the other measures, they are mutually incompatible.

Trying to cover all aspects of high scientificity suffers from the short blanket syndrome. It is like trying to achieve a high yield, selective, cheap and environmentally friendly synthesis, all together. It will just not happen; we know it and we accept it. Sacrifices are to be made, or that paper will never see the light. We can conceive a "soft hypersphere" model (Fig. 1), where on each axis we have different scientificity properties. We try to go as far from the centre as possible, since in the centre we are in the pseudoscience nucleus; the largest the radius, the higher the scientificity level. However, at certain point we find it more and more difficult to advance beyond the blurred scientificity frontier, a zone where we can only find what we might consider science fiction.

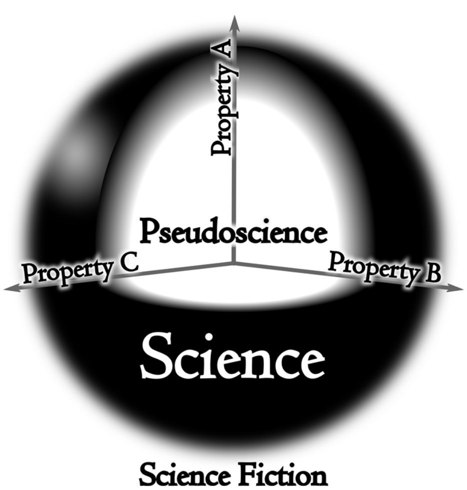


Figure 1. The soft hypersphere scientificity model. It is impossible to achieve high scientificity on every aspect of science, since some properties are, to some extent, mutually exclusive. However, as long as we stay close to the surface, there are many ways to do it.

Speaking about geometrical analogies, we can try to guesstimate the distribution of science and pseudoscience practitioners. These numbers are hard to obtain, and as far as I know nobody did such statistics. An old estimate postulated that for every astronomer in the US there are ten astrologers. However, trying to find this ratio sounds like a wild-goose chase, since there are many types of astronomers (PIs, grad or undergrads, citizen-astronomers, cosmologists, exobiologists, astrochemists, etc.) and astrologers (Chinese, western, vedic, zodiac, natal charting, newspaper horoscope quacks, amateur couch astrologers, etc.). But we can still make some overgeneralizations based on some weak deductive reasoning.

From all the chemistry researchers that we know, we may say that the large majority are working well within the parameters of high scientificity (at least most of the chemists I know). Doing progressive research is extremely demanding, research positions are not abundant, grants are also not exactly generous, and publishing usually requires passing the reviewers' filter. That produces a self-correcting system making most researchers and their projects fit into a narrow distribution of high scientificity. We all know one or two outliers from both sides, someone doing incredible chemistry with high insight, predictions, discoveries and progress, and someone doing lousy chemistry which hardly deserves to be published. But most of us are just simple, law-abiding chemists.

On the other side, most pseudosciences will never pass the bare minimum of the scientificity requirements. For sure they are not progressive, and they are either non-falsifiable or already falsified (as someone said: "How do you call the alternative medicine that has been proven to work? Medicine!"). But be aware that pseudosciences can comply with some rules, like following natural laws. Most of those "laws" would make us cringe, like the laws for classical elements (water-fire-air-earth, or wood-metal-fire-water-earth, or sulphur-mercury-salt, etc.), or the law of similarities in homeopathy, or, heaven forbid, even the law of attraction. Dreadful laws, but still laws. Bear in mind that, oppositely, some aspects of science are barely based on any law, like discovering a new fungus or comet, or using combinatorial chemistry (forgive my heresy), so in this aspect it is easy to fall in the epistemological trap of making inflexible demarcation rules.

Sometimes a pseudoscientific trait consists in taking lessons from science but not applying them in a scientific manner. This is like doing the above cited "resemblance thinking" in a kind of cargo cult. For instance, homeopathy wrongly takes chemical principles at face value, without really testing the validity of their postulations. Taking real scientific ethics is very costly in terms of time, money and cognitive efforts, and therefore whoever is doing pseudoscience will be ill-disposed to follow that path. Nevertheless, at a certain point even pseudoscientists are disinclined to follow the path of completely going against reality. Homeopaths and new age environmentalists still believe that the world is not flat or dominated by reptilians, and most of them even believe that humans reached the moon. Therefore, most pseudoscience is also unified into a narrow distribution, but in this case of low scientificity.

If we were able to do statistics, what we would possibly see is a bimodal distribution (Fig. 2) of work styles and ethics. Between them we may find a small population doing what someone called "fringe science". While string theory is often cited as fringe science, the pet model for fringe chemistry is cold fusion: the possibility of having nuclear hydrogen fusion at room temperature, especially by electrochemical procedures. The topic was reborn in 1989 with great fanfare, after which it had a very bumpy ride and deep fall. Even if scientists are very sceptical, brave researchers are still trying to resurface the field.[26] Note that besides "fringe science" there are terms for other borderline approaches with much worse reputation, such as the "bad science" typical of bad pharma,[25] "pathological science", "junk science", "fake news science", "predatory science"… but all these definitions are material for another article.

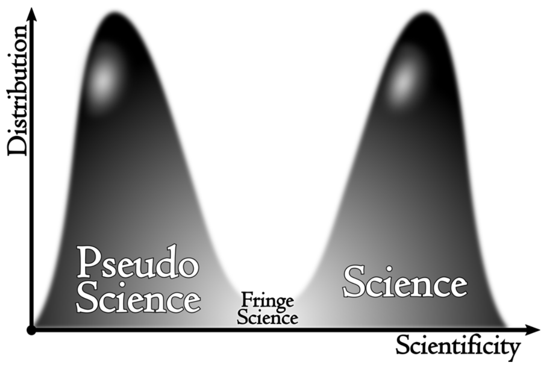


Figure 2. The model bimodal scientificity distribution. Most scientists know the epistemological limits of science, and most pseudoscientists know the cost of raising the bar, producing a buffer zone between them.

This shows that there is some scientific mobility, which must be taken as part of the scientific universe. Also, the rules of science may slowly change (we certainly do not see the world through the same eyes of the Renaissance man), and whatever I believe to be the greatest rules of science may not be the preferred scientific priorities of my fellow chemist. Scientificity is a very subjective measure, a continuous and blurred distribution somewhat connected to the "everything goes" maxim.

On the Nature of The Supreme Scientificity Demon, or How we can Keep Track of the Future

Let us imagine a scientific demon that can practice research with 100% scientificity on every aspect that characterizes science. Progressiveness? Check. Explanatory and predictive power? Check. Falsifiability? Absolutely. Empirical tests that would make Hume blush? Sure. Stronger deductive powers than Sherlock Holmes? No problem. Coherence and consistency in front of any and all natural laws? Bring it on!

What would make such a demon? How would it know that, for instance, the catalyst that it is developing has a much higher rate of reaction than any other catalyst for the same reaction, that it will pass every one of the infinite possible kinetic tests, that it can be explained and reduced to all the known chemical laws (Eyring, Jahn-Teller, $\hat{H}\Psi$, you name it), be predicted to produce absolute enantiomeric excess, and even generate a scientific revolution in the catalytic community? My humble guess is that such demon must have similar qualities to Laplace's demon: "*for such an intellect nothing would be uncertain and the future just like the past would be present before its e*yes". Our demon must probably be omniscient! There is only one problem: if such demon exists, it does not need to do science, since science deals with the unknown, and the unknown is unknown to the demon. Or as the quote wrongly attributed to Einstein says: "*If we knew what we were doing, it wouldn't be called research, would it?*"

But there is one system that many scientists exploit to resemble our scientific demon. Simply have several projects, one with high certainty but a low progressiveness chance, one highly risky but potentially revolutionary, one working on an emergent field of an emergent property, one firmly based on reducing laws… It is impossible to break out of the scientificity hypersphere, but it is possible to cover all of its surface with different research projects. Or as a chemist told once, "give your student one easy and one hard project; they may or may not generate a breakthrough, but at least they will have a thesis".

On the Nature of the Usefulness of Philosophy of Science for Chemistry, or How to Justify such Philosophical Endeavour

Is Philosophy of Science useful for chemists?

No.

In a round-table debate about the usefulness of philosophy of science, it was memorably claimed that *"Scientists are very ambitious. They're very competitive. If they really thought philosophy would help them, they'd learn it and use it. They don't."*[27]

In a recent opinion article on why science needs philosophy,[28] many examples of the interaction between state of the art philosophy of sciences and specific research projects were depicted. But to be honest, these look more like cherry picking the small number of existent shared philosophy-science projects than to a general state of affair. I am certain that most of the most successful chemists have never interacted with a philosopher in their lives, and they probably do not regret it.

However…

Philosophy of science and philosophy of chemistry in particular are putting a magnifying glass over us. Wouldn't you be interested in knowing what they see? Maybe it is a good idea to practice a bit of metacognition, to think about how we think, to have some introspection about how and why we do chemistry, and what justifies our chemical reasoning. You can live a good and fruitful life without knowing that you have a brain, but it is not something to be proud of. Or as the maxim engraved in the forefront of the temple of Apollo at Delphi teaches us, γνῶθι σεαυτόν ("Know Thyself"). We should not work on automatic mode, we must try to understand the weaknesses and strengths of the chemical way. If we have a chemical identity crisis, it is always good to have a philosopher friend. Who knows, they might appreciate speaking with a chemist as well.

Now it is farewell time, after a longer than expected article. While you may justifiably criticize that most of this article's topics were only touched in an extremely superficial way, you can criticize even more that there are many aspects of philosophy that were left completely out from this article: popular science and scientific journalism, chemical education, a real discussion on serendipity, scientific literature and publications, realism and naturalism, chemistry vs. other sciences, creativity in chemistry, beauty in chemistry, chemical holism, foundations of chemistry, chemical ethics, chemical sociology and history, junk chemistry, meta-chemistry, and my favourite, philosophy of theoretical and computational chemistry,[29] among many other topics. But conciseness is another good trait of science, therefore this is a good point to wrap it up. We will only conclude that from a scientificity point of view, chemistry is good.

For the last paragraph, let me just plagiarize the last paragraph of Berson's "Chemical discovery" book:[17]

"*The progress of chemistry, and I believe, of most of science, takes place in a contexture of chaos. Scientific knowledge grows despite illogicality of the means by which it has been acquired, despite scientists' clumsiness in manipulating the tools of proper* *inference… Is there an alternative pathway to the one we had planned, one which is not yet on any map, one which is more direct and which expands the scope of our vision far beyond our expectation? Are there new goals we have not yet discerned that we should be trying to reach? If philosophers can help us to find such trails, scientists will welcome them with open arms as companions on the quest.*"

1 Reviewer 2 Must Be Stopped! (Facebook Group), https://www.facebook.com/groups/71041660468/, (accessed 3 August 2020).
2 M. Curd and J. A. Cover, Eds., *Philosophy of science: the central issues*, W.W. Norton, New York, 1st ed., 1998.
3 P. Godfrey-Smith, *Theory and reality: an introduction to the philosophy of science*, University of Chicago Press, Chicago, 2003.
4 S. Okasha, *Philosophy of science: a very short introduction*, Oxford University Press, Oxford ; New York, 2002.
5 K. R. Popper, *The Logic of scientific discovery*, Routledge, London, 2009th edn., 1935.
6 D. Wu, K. Kusada, T. Yamamoto, T. Toriyama, S. Matsumura, S. Kawaguchi, Y. Kubota and H. Kitagawa, Platinum-Group-Metal High-Entropy-Alloy Nanoparticles, *J. Am. Chem. Soc.*, 2020, **142**, 13833–13838.
7 *Personal communication. February 2016*.
8 T. S. Kuhn, *The structure of scientific revolutions*, The University of Chicago Press, Chicago ; London, Fourth ed., 2012.
9 I. Lakatos and A. Musgrave, Eds., *Criticism and the growth of knowledge*, University Press, Cambridge [Eng.], 1970.
10 The Solar Army | NSF Center for Chemical Innovation in Solar Fuels, https://thesolararmy.org/, (accessed 30 July 2020).
11 G. Russell, in *Martial Arts and Philosophy*, eds. G. Priest and D. Young, Chicago and Lasalle, Illinois: Open Court, 2010, pp. 129–144.
12 HYLE--International Journal for Philosophy of Chemistry, http://www.hyle.org/, (accessed 29 July 2020).
13 Foundations of Chemistry, https://www.springer.com/journal/10698, (accessed 29 July 2020).
14 E. R. Scerri, *Collected papers on philosophy of chemistry*, Imperial College Press, London, 2008.
15 A. Woody, R. F. Hendry and P. Needham, Eds., *Philosophy of chemistry*, Elsevier/NH, North Holland is an imprint of elsevier, Amsterdam ; Boston, First edition., 2012.
16 J. van Brakel, *Philosophy of chemistry: between the manifest and the scientific image*, Leuven University Press, Leuven, 2000.
17 J. A. Berson, *Chemical discovery and the logicians' program: a problematic pairing*, Wiley-VCH, Weinheim, 2003.
18 R. Hoffmann, J. Kovac and M. Weisberg, *Roald Hoffmann on the philosophy, art, and science of chemistry*, Oxford University Press, New York, 2012.
19 Jargonium - A blog about chemistry, https://www.jargonium.com/, (accessed 27 November 2020).
20 V. Seifert, Strong Emergence in Chemistry, https://www.jargonium.com/post/strong-emergence-in-chemistry, (accessed 29 November 2020).
21 P. Schwerdtfeger, O. R. Smits and P. Pyykkö, The periodic table and the physics that drives it, *Nature Reviews Chemistry*, 2020, **4**, 359–380.
22 E. R. Scerri, *The periodic table: its story and its significance*, Oxford University Press, New York, NY, 2nd ed., 2019.
23 P. Thagard, *Computational philosophy of science*, MIT Press, Cambridge, Mass, 1988.
24 P. Feyerabend, *Against method*, Verso, London ; New York, 3rd ed., 1993.
25 B. Goldacre, *Bad pharma: how drug companies mislead doctors and harm patients*, Fourth Estate, London, 2012.
26 J.-P. Biberian, *Cold fusion: advances in condensed matter nuclear science*, Elsevier, Amsterdam, Netherlands, 2020.
27 Round Table Debate: Science versus Philosophy? | Issue 27 | Philosophy Now, https://philosophynow.org/issues/27/Round_Table_Debate_Science_versus_Philosophy, (accessed 30 July 2020).
28 L. Laplane, P. Mantovani, R. Adolphs, H. Chang, A. Mantovani, M. McFall-Ngai, C. Rovelli, E. Sober and T. Pradeu, Opinion: Why science needs philosophy, *PNAS*, 2019, **116**, 3948–3952.
29 R. Hoffmann and J.-P. Malrieu, Simulation vs. Understanding: A Tension, in Quantum Chemistry and Beyond. Part A. Stage Setting, *Angew. Chem. Int. Ed.*, 2020, **59**, 12590–12610.