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Why Do Chemists Perform Experiments?

Introduction

Nowadays it is well known among historians of science that Francis Bacon, one of the modern defender of the experimental method, owed much of his thoughts to the chemical or alchemical tradition (cf. e.g., Gregory 1938, West 1961, Linden 1974, and Rees 1977). In fact, alchemy, particularly in the Arabic tradition, was always based on laboratory investigations by carefully examining the results of controlled manipulation of materials.[1]

It is also well known that Francis Bacon's appeal to the experimental method was severe criticism of scholasticism in philosophy of nature and, in particular, of authority as the basis of knowledge.[2] If we compare philosophy of nature in the early 17th century with phi-

[1] As Newman (1998) has argued, and as some essays published in the same volume as Newman's essay exemplify it again, both philosophers and historians of physics have stubbornly denied this fact.

[2] "Verum dum opinionibus et moribus consulitur, mediocritates istae laudatae in magnum scientiarum detrimentum cedunt" (*Novum Organum*, Praefatio [*Works*, Spedding & Ellis, vol. I, p. 128]).

losophy of science in the 20th century, several similarities appear. Not only does much of the language orientation in philosophy of science resembles scholastic approaches; the way they refer to classics, such as Carnap, Reichenbach, Hempel, Popper, Kuhn, Feyerabend, and the like, also show gestures of bowing to authority. Moreover, the recent shift from philosophy of science toward *history* of philosophy of science indicates, in my view, a crisis of the whole discipline.

Francis Bacon's remedy against intellectual ossification was fresh empirical input. That was explicitly not meant as a basis for logical induction,[3] as many have misunderstood him later. To the contrary, Bacon strictly rejected what he called Aristotelian induction throughout his writings. Instead, empirical data should help develop new hypotheses about nature, which in turn should encourage new experiments, and so on. The remedy was meant to avoid blind speculations on nature and to undermine ossified fictions. Rather than providing a logical basis for induction, it should provoke and challenge the scholastic tradition and prepare the grounds for innovations.

In this paper, I follow the Baconian approach by empirically investigating science instead of nature. I provide some empirical results about what chemists are actually doing. In particular, I shed some light on what chemists mean by 'experiment', how they do experiments, and why they do that.[4] The quantitative results are based on various document analyses of several hundred chemical papers, randomly selected from two chemistry journals. The results, which are statistically qualified, should not be considered a logical basis for induction, but simply a starting point for philosophical reflection about science. In addition, they are meant to provoke traditional ways of doing philosophy of science.

[3] "Inductio enim quae procedit per enumerationem simplicem res puerilis est, et precario concludit, et periculo exponitur ab instantia contradictioria, et plerumque secundum pauciora quam par est, et ex his tantummodo quae praesto sunt, pronunciat" (*Novum Organum*, I.105 [*Works*, Spedding & Ellis, vol. I, p. 205]).

[4] For a broader conceptual analysis of the various roles of experiments in chemistry, as opposed to the notion of experiment in the philosophy of physics tradition, see Schummer 1994.

1. A quantitative look at the sciences

Let us first have a quantitative look at the activities of the sciences as indicated by the number of publications indexed by their corresponding abstract journals (Fig. 1).

Surprisingly, chemistry is not only the biggest science, it is even bigger than the total of all the other natural sciences including their various related technologies which, like computer science, information technology, and biotechnology, greatly flourished during the past two decades. Thus, if we want to know what our actual sciences are about, we should – from a quantitative point of view – first and foremost turn our attention to chemistry. Or, to put it in different terms, philosophies of the natural sciences that neglect chemistry should arouse our strongest suspicion. Moreover, chemistry has always been the laboratory science *per se*, such that still in the 19th

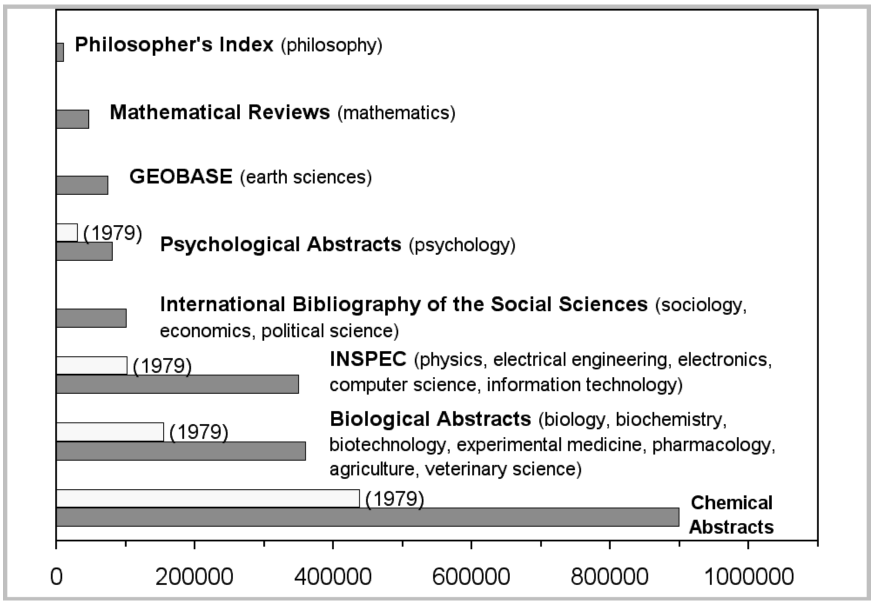

Fig. 1. Number of new publications (papers, patent, books, etc.) indexed by the major abstract journals in 2000 and 1979, respectively. Data from Schummer 2003 and Tague et al. 1981

century the term 'laboratory' denoted a place for experimental research in which *chemical* operations were performed (Nye 1993, p. 50). The chemical laboratory became the model for all the other laboratory sciences when they replaced 'thought experiments' by real experiments. Although chemistry is no longer the only experimental science, it is by far the biggest one and historically the model for all others. Thus, if we want to know what scientists mean by 'experiment', chemical papers are the right point to start with.

2. Chemical experiments: synthesis and analysis[5]

According to some mainstream ideas of philosophy of science, scientists invent and test new theories. If by deductive reasoning a theory predicts a certain event to happen in certain circumstances, it is the experimenter's task to skillfully develop a corresponding laboratory setting and to check whether the event actually happens as predicted by the theory or not. Experiments, in this view, are nothing else than tools for quality controls of theoretical knowledge.[6] They help prevent our ideas about nature from loosing contact with 'empirical reality'.

Let us now test that philosophy of science hypothesis by confronting it with some empirical data. Today there are about 4 million chemists worldwide producing some 900,000 papers a year. Because about two thirds of these papers report on the synthesis and analysis of new substances, it is fair to say that the synthesis and analysis of new substances are the main laboratory activities of chemists. In 2001, they made about 1.6 million new ones – if one includes biosequences, it was even 6.75 million. Figure 2 presents a survey of chemical substance productivity during the past 200 years. The numbers are collected from various handbooks, such as *Beilstein*, *Gmelin*, and *Chemical Abstracts*.

[5] This section is based on empirical studies published in Schummer 1997a/b and on updated data from Chemical Abstract Service 2002.

[6] I skip here the rather obscure, albeit widespread, opinion that experiments necessarily include measurements and ignore all views that implicitly consider classical astronomy an experimental science.

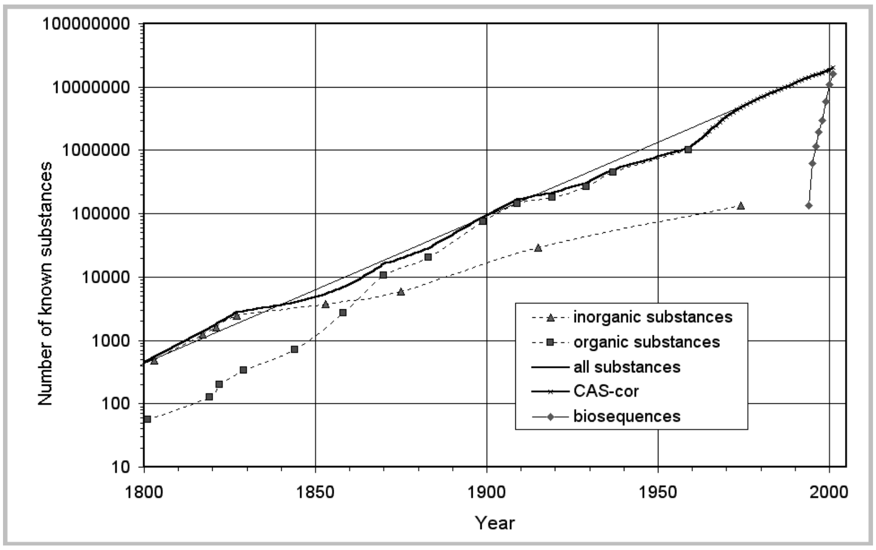

Fig. 2. Growth of chemical substances. Data from Schummer 1997a and Chemical Abstract Service 2002

Note that the figure has a semi-logarithmic scale. The bold line is the growth of all chemical substances. There is nearly stable exponential growth during the whole period, with annual growth rates of about 5.5% and doubling times of 13 years (the straight line is a fit to the last 20 years). Deviations are largely due to war effects. Also note that some 95% of all known substances are artifacts, i.e., they are not found in 'nature' by simple isolation.

Producing new substances is, for sure, not the only activity of chemists. Analytical chemists improve analytical methods, quantum chemists try to solve Schroedinger equations, physical chemists measure chemical reactions, technological chemists develop and improve new industrial processes, and so on. However, the great majority of chemists actually produce new substances. That is by far the largest scientific enterprise – roughly estimated, a third of all scientists worldwide are involved in this project. Surprisingly, no philosopher of science seems to have ever been aware of it.

If we want to know what chemists mean by 'experiment', nothing is simpler than that. Every paper has a section called 'Experimental'.

In that section, chemists first describe in detail how they have made their new substances. Second, they provide various properties of the new substances including the corresponding experimental methods. Thus, performing experiments largely comprises two activities: (1) performing chemical reactions in order to form new products, including their isolation and further processing; (2) investigating various properties of the new products. That is exactly the couple of experimental (not conceptual!) *synthesis and analysis*, which is indeed as old as chemistry.

As mentioned above, philosophers of science are used to consider experiments as related to theory in one or the other way. Let us see if we can find something like that by having a closer look at *how and why* chemists both produce new substances and investigate their properties.

3. How and why do Chemists Investigate Properties of new Substances?

The investigation of properties of substances, including their elemental composition, is what chemists usually call analysis. With few exceptions, they have followed standard procedures whenever the objects of investigation have been *new* substances.[7] From the early 19th century to the 1960s, there was virtually a *canonical characterization* that included the following items:

1) results of elemental analysis incl. empirical formula (occasionally molecular weight);

2) melting point or boiling point (incl. pressure if vacuum distillation was applied);

3) visual characteristics (crystal form, color);

4) solubility in various solvents;

5) some exemplary statements about chemical reactivities.

The canonical characterization was simply meant *to determine the identity of the new substances*. As I have argued elsewhere (Schummer 2002), that approach became insufficient when it failed to clearly distinguish hundreds of thousands of substances from each other. The

[7] This section draws on empirical results from Schummer 2002.

main support for determining substance identity came from chemical structure theory.

Nowadays we are inclined to consider structure theory only a step into the microcosm of molecules. Such a view, however, overlooks the specific needs of chemists, namely to cope with the issue of species identity when the number of substances to be clearly distinguished grew to millions. The theoretical notion of molecular structure was an ingenious solution in that regard. Instead of collecting arbitrary sets of empirical properties, chemists explored certain chemical properties that helped assign a molecular structure to each substance in an unambiguous way. For the purpose of the present paper, it is important to note that theory, here classical chemical structure theory, played only an instrumental role for the ontological issue of substance identity: substance identity was determined by structure identity. From a pragmatic point of view, it was just a theoretical guide to select as many characteristic material properties as needed for fixing substance identity.

With the raise of spectroscopic instrumentation since mid-20th century, structure determination by chemical properties was gradu-

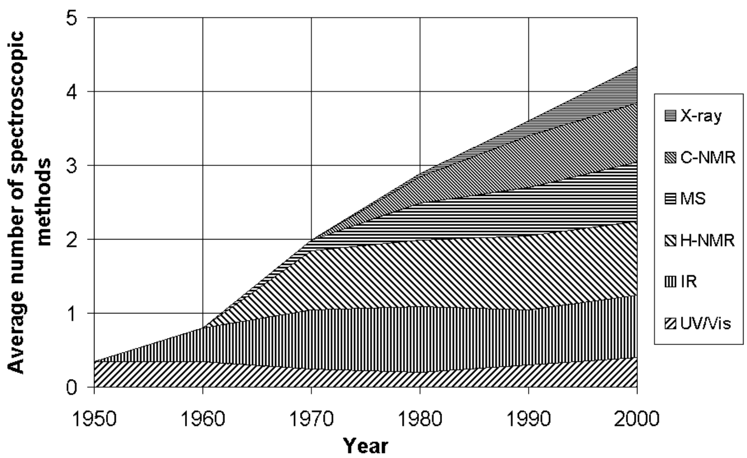

Fig. 3: Average number of spectroscopic methods (incl. X-ray diffraction) used for the characterization of new solid organic compounds in papers of *Liebigs Annalen* (2000, *European Journal of Organic Chemistry*). Data from Schummer 2002

ally replaced by spectroscopic data (Fig. 3). The basic approach remained the same, however. Chemists collected as many spectroscopic data, i.e. optical properties, as needed for an unambiguous structure determination. Only the sort of structure changed, from constitutional to configurational structures, and more recently to conformational structures. Along with this shift, the number of applied spectroscopic methods grew, as well as their technological refinements.

The main purpose of investigating material properties of new substances, immediately after their first synthesis, has always been the same. The new products need to be characterized in an unambiguous way, such that each chemist can claim the identity of his or her creation. To that end, structure theory has been an extremely useful tool. In addition, spectroscopic methods have required theoretical analysis of data on an increasingly sophisticated theoretical level of quantum chemistry. Yet, any such use of theory in experimental analysis has always been instrumental to the aim of analysis.

4. How do chemists make new substances?

Let us now turn to the synthesis part of chemical experiments.[8] How do chemists make new substances? In particular, what role does theory play in the planning and preparation of synthetic experiments? Is the outcome of these experiments even predicted by theory?

To answer these questions I have analyzed 300 papers searching for any clues by the authors. The papers were classified according to six categories:

(1) no statements about instructions;

(2) the new substance is made without instruction, indicated by terms like "surprisingly", "contrary to expectations", "by chance";

(3) preparation is carried out by analogy with a former preparation of one of the authors according to a reference ("self-analogy");

(4) preparation is carried out by analogy with a former preparation of a different author according to a reference ("other analogy");

[8] This and the following sections draw on empirical results from Schummer 1997b.

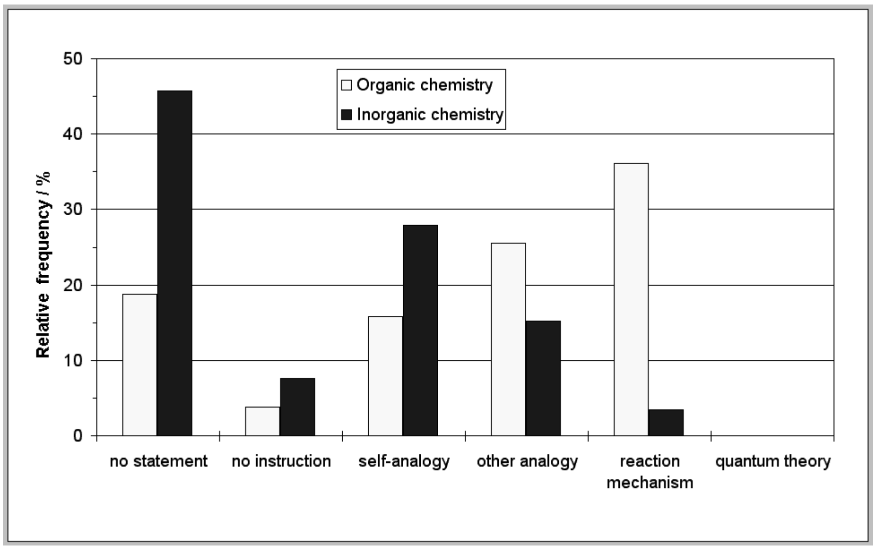

Fig. 4: Instructions for making new substances, 300 journal papers of the years 1980–1995 considered. Data from Schummer 1997b

(5) preparation is planned (not reconstructed) on the theoretical level of reaction mechanisms;

(6) preparation follows predictions of or clues from quantum chemical models.

What strikes first is that there is a big difference between organic and inorganic chemistry. Without going into details, we can say that inorganic chemists largely work without explicit instructions, i.e. either by some intuitive access or by a combinatoric trial and error approach or by analogy with what they personally did before. Organic chemists, on the other hand, are largely guided by reaction mechanisms.

Another surprising fact is that, despite the weight given by philosophers of science, quantum mechanics provides no predictions of chemical synthesis experiments, at least nothing that would be measurable by statistical methods. Indeed, none of the 300 papers refers to any quantum theoretical clues for the synthesis of a new substance. If we are looking for the role of theory in synthesis experiments, we must address reaction mechanisms, which indeed play a pivotal role in organic chemistry. Yet, instructions from reaction mechanisms are also a kind of analogy on a theoretical level. As every chemist knows, the planning of a new synthesis is no simple deductive reasoning. If that were the case, it would lose any scientific value for chemists. Even more, chemistry journals do not accept papers about easily predictable experimental results. Purely deductive approaches like the synthesis of biosequences are made by automata and not by working scientists. Instead, emphasis is on the unforeseeable, the innovation.

Overall, reaction mechanisms have tremendously predictive power regarding the synthesis of new substances. Yet, in chemistry such predictions are rarely made to test a theory (see below), but to provide instructions for chemical synthesis. Rather than being tools for deductive reasoning, reaction mechanisms provide sets of theoretical possibilities that need to be carefully combined and adapted to certain instances of experimental synthesis. In chemical synthesis, like in any truly experimental research, experiments are not tools for evaluating theories – instead, theories are tools for research experiments, tools for exploring the new.

5. Why do chemists make new substances?

The synthesis of new substances is a major part of experimental research in chemistry. Since research aims at exploring new fields of knowledge, the question arises as to what kinds of cognitive objectives chemists follow when they proliferate the number of known substances. A random sample survey of 300 papers of one of the most important international journals in general chemistry (*Angewandte Chemie*) should provide a fairly representative and statistically qualified answer. In fact, journals in general chemistry, like *Angewandte Chemie*, require that authors in their papers provide reasons why their particular research is of general concern and interest. Although such explicit research reasons may occasionally differ from personal motives, these are acknowledged aims of the research community. Figure 5 presents the distribution of such aims based on a document analysis of the mentioned sample.

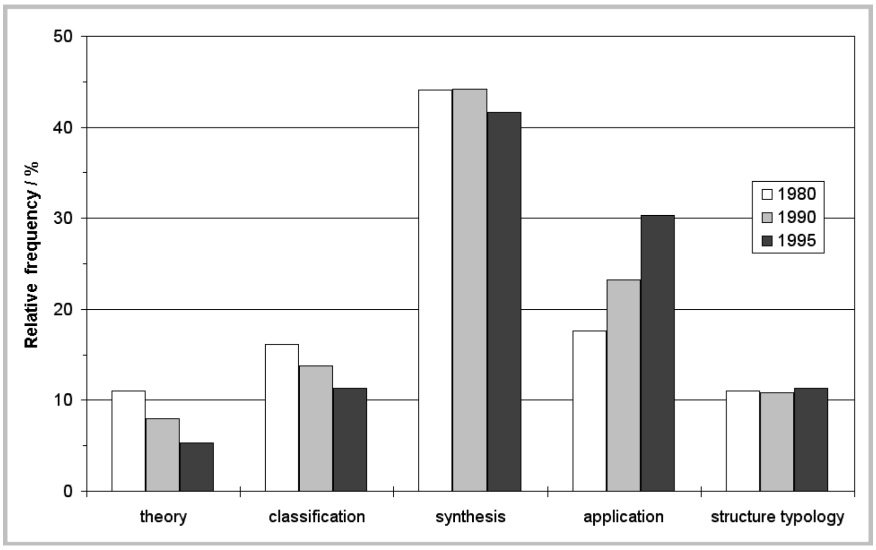

Fig. 5. Relative frequencies of aims in synthetic chemistry, 300 journal papers of the years 1980–1995 considered. Data from Schummer 1997b

The aims are divided into 5 groups. The first group, *theory*, contains everything philosophers of science have told us why experiments are performed in science: the confrontation of theories with experimental results for testing, exhausting, refining theories, models, and so on. Obviously, theories are not very important in chemistry. A bit more important are questions concerning *classification*, *e.g.*, the development of new substance classes, undermining former classificatory distinctions, and so on. Today's chemists also have a considerable fable for *structural features* of their substances (strange angles, unusual symmetries, and so on), which is difficult to understand from the outside of chemistry and which is different from aims of the theory group. More important, however, are the two remaining groups. The *application* group includes the search for new materials that might be of practical or technical use, *e.g.*, in pharmacy, agriculture, electroengineering, and so on. Although applied research is of considerable and increasing importance in chemistry, it is by no means the first goal. Instead, the great majority of synthetic research is performed to improve the synthetic abilities of chemistry itself. The *synthesis* group contains the production of new important reagents or catalysts and the development of new general synthetic methods both on the empirical level of recipes and the theoretical level of reaction mechanism.

A most striking result, nearly half of the production of new substances is in order to improve the abilities to produce more new substances. That is, producing new substances is actually an end in itself for the whole field, albeit not for each individual synthesis – and it is an extremely successful one as the exponential growth of substances demonstrates (Fig. 2).

We are now in the position to reconsider the part of theory in synthetic experiments. The explicit aim of exploring reaction mechanisms is to improve synthetic abilities. Note that the instrumental status of theories is not the outcome of removed philosophical interpretation, as part of the realism/instrumentalism debate in philosophy of science. Instead, it is what chemists actually say and do. Moreover, the instrumental status of reaction mechanisms has nothing to do with a technological interpretation of science. Instead, theory is considered a tool for chemical experiments, and not the other way round.

6. Conclusion

Based on several empirical analyses I have shown that in chemistry

(1) 'experiment' for the most part means synthesis and analysis of new substances;
(2) analysis, i.e. investigating material properties, aims at determining substance identity;
(3) theory is instrumental in analysis, by selecting and interpreting material properties in order to determine substance identity at the structural level;
(4) synthesis largely aims at improving synthetic abilities;
(5) theory (classical reaction mechanisms) is instrumental in synthesis, by guiding synthesis through analogies at the structural level.

As a result, we have a methodological sketch of synthetic chemistry that I consider only a preliminary result, as a starting point to develop a deeper understanding of chemistry by philosophical reflection. At the present state, however, it seems to be already clear that our results do not fit in any of the traditional accounts of philosophy of science. For instance, no philosopher did ever mention the synthetical and analytical objectives of experiments,[9] despite the fact that the majority of scientists have just that in mind. By putting too much emphasis on the epistemological side, methodologists of science continue to overlook that scientists do not simply describe the world as it is, but mainly create new entities. In the experimental sciences, experiments are no epistemic tools for checking theories; instead theories are instruments for guiding experiments. While the exact role of theories is still less understood, it seems to be already clear that they are not used for simple deductive reasoning in chemistry. In analytic experiments they help determine substance identity by interpreting empirical properties. In synthetic experiments they rather serve as a pool for drawing analogies on a theoretical level.

Finally, let us consider why mainstream philosophers of science might have neglected all that, despite the fact that we are dealing here with the by far largest part of the experimental sciences. I suspect that philosophers tend to rely on three evasive approaches.

(1) One way to disregard chemical experiments is by applying the *distinction between science and technology*. If chemists are largely producing new substances, this shall be taken as technology and not as science. As I have argued in detail elsewhere (Schummer 1997), that strategy does not work. In particular, producing new entities does not suffice to call that activity technology. A closer look at all the famous distinctions between science and technology, as put forward from Aristotle up to the present, shows that all of them are outdated, one-sided, or arbitrary. At best such distinctions can arbitrarily select

[9] In fact, mainstream philosophy of science is so removed from the actual experimental sciences that philosopher Michael Heidelberger (1998) needed to take great pains to point out the explorative role of experiments.

some 5 % of physics as the only 'real science' per definition, in contrast to what is usually considered science.

(2) A second evasive approach is applying the *distinction between the context of discovery and the context of justification*. One could say that chemical experiments of synthesis and analysis belong only to the context of discovery. In some sense that is true, if it means the discovery of new substances, their properties, and production methods, instead of the discovery of theories. However, note that the analysis of aims as presented in Section 5 covers both contexts as different aims. As a matter of fact, it turns out that chemists are not much interested in justifying their theoretical concepts by experiment. Since they do not use them for universal description of the world but as tools, they probably have different approaches to make them reliable for their particular purposes.[10] In other words, since it is unclear what 'context of justification' should exactly mean in chemistry as well as in most other sciences, the whole distinction is questionable.[11]

(3) One could also say that what I have emphasized with reference to empirical analyses are just the *philosophically uninteresting* parts of chemistry. Synthesis and analysis of new substances are parts of everyday chemistry, whereas the highlights of chemistry are to be found in quite different regions, such as in recent trends in quantum chemistry or in biochemical attempts to explain life. Here, we actually come to the core of the issue: what is the meaning of 'being philosophically interesting'? I suspect that this term simply refers to what received philosophers of science (largely of physics) considered to be interesting; that is to say, 'interest' is a culturally embedded notion related to the objectives of (the philosophical caricatures of) physics.[12] As a con-

[10] See Schummer 1998.

[11] From the philosopher's point of view it is even worse, since the whole notion of confronting theories with experiments is nearly absent here: If chemists, particularly inorganic chemists, are discussing structures of their new substances, they refer to spectroscopic measurements in the very same way as they refer to quantum chemical calculations, as long the data help assign an unambiguous structure. Rather than validating theoretical concepts, these concepts are applied to solve particular chemical problems if they are useful; otherwise they are modified or adapted.

[12] See also Schummer 2003, sect. 1.

sequence, if one looks upon chemistry from the traditional point of view, nearly everything of chemistry turns out to be uninteresting. However, that simply means that chemistry is different from the philosophical sketches of physics, and that chemists follow different aims and use different methods than physicists.

Whatever kind of strategy philosophers of science might apply to ignore the major part of the actual sciences, the prize is very high: it is the lack of understanding of what the majority of scientists are doing. We are just at the beginning to understand these activities, for which the empirical analyses are only preliminary studies. If it is our goal, as philosophers of science, to understand the actual sciences, then we need to address these issues – whether we like it or not.

References

Bacon F. (1857ff.). *The Works of Francis Bacon*. 14 Vols. Ed. J. Spedding. London: Longman, 1857–1874.

Chemical Abstract Service (2002). *Statistical Summary 1907–2001*. Columbus, Ohio.

Gregory J.C. (1938). "Chemistry and Alchemy in the Natural Philosophy of Sir Francis Bacon, 1561–1626". *Ambix*, **2**, pp. 93–111.

Heidelberger M. (1998). "Die Erweiterung der Wirklichkeit im Experiment". In: M. Heidelberger & F. Steinle (eds.), *Experimental Essays – Versuche zum Experiment*. Baden–Baden: Nomos, pp. 71-92.

Linden S.J. (1974). "Francis Bacon and Alchemy: the Reformation of Vulcan". *Journal of the History of Ideas*, **35**, pp. 547–560.

Newman W. (1998). "The Place of Alchemy in the Current Literature on Experiment". In: M. Heidelberger & F. Steinle (eds.), *Experimental Essays – Versuche zum Experiment.* Baden–Baden: Nomos, pp. 9–33.

Nye M.J. (1993). *From Chemical Philosophy to Theoretical Chemistry*. Berkeley: University of California Press.

Rees G. (1977). "Matter Theory: a Unifying Factor in Bacon's Natural Philosophy?". *Ambix*, **24**, pp. 110–125.

Schummer J. (1994). "Die Rolle des Experiments in der Chemie". In: P. Janich (ed.), *Philosophische Perspektiven der Chemie*. Mannheim: Bibliographisches Institut, pp. 27–51.

Schummer J. (1997a). "Scientometric Studies on Chemistry I: The Exponential Growth of Chemical Substances, 1800–1995". *Scientometrics*, **39**, pp. 107–123.

Schummer J. (1997b). "Scientometric Studies on Chemistry II: Aims and Methods of Producing New Chemical Substances". *Scientometrics*, **39**, pp. 125–140.

Schummer J. (1997c). "Challenging Standard Distinctions between Science and Technology: The Case of Preparative Chemistry". *HYLE – International Journal for Philosophy of Chemistry*, **3**, pp. 81–94.

Schummer J. (1998). "Physical Chemistry: Neither Fish nor Fowl?". In: P. Janich & N. Psarros (eds.), *The Autonomy of Chemistry*. Würzburg: Königshausen & Neumann, pp. 135–148.

Schummer J. (1999). "Coping with the Growth of Chemical Knowledge: Challenges for Chemistry Documentation, Education, and Working Chemists". *Educación Química*, **10**, pp. 92–101.

Schummer J. (2002). "The Impact of Instrumentation on Chemical Species Identity: From Chemical Substances to Molecular Species". In: P. Morris (ed.), *From Classical to Modern Chemistry: The Instrumental Revolution*. Cambridge: Royal Society of Chemistry, pp. 188–211.

Schummer J. (2003). "The Philosophy of Chemistry: From Infancy Towards Maturity". In: D. Baird, E. Scerri, L. MacIntyre (eds.), *Philosophy of Chemistry: Synthesis of a New Discipline* (Boston Studies in the Philosophy of Science series), Dordrecht: Kluwer (in preparation).

Tague J., Beheshti J. & Rees-Potter, L. (1981). "The Law of Exponential Growth: Evidence, Implications, and Forecasts", *Library Trends*, **30**, pp. 125–150.

West M. (1961). "Notes on the Importance of Alchemy to Modern Science in the Writings of Francis Bacon and Robert Boyle". *Ambix*, **9**, pp. 102–114.