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Coping with the Growth of Chemical Knowledge

Challenges for Chemistry Documentation, Education, and Working Chemists

Joachim Schummer

Institute of Philosophy, University of Karlsruhe, D-76128 Karlsruhe, Germany,
Joachim.Schummer@geist-soz.uni-karlsruhe.de

Abstract: Chemistry is by far the most productive science concerning the number of publications. A closer look at chemical papers reveals that most papers deal with new substances. The rapid growth of chemical knowledge seriously challenges all institutions and individuals concerned with chemistry. Chemistry documentation following the principle of completeness is required to schematize chemical information, which in turn induces a schematization of chemical research. Chemistry education is forced to seek reasonable principles of selectivity, although nobody can have an overview any more. Philosophical evaluation of the growth of chemical knowledge proves that at the same time chemical 'nonknowledge' increases more rapidly. An analysis of reasons, why chemists are making new substances at all, shows that the proliferation of new substances is for the most part an end in itself. The present paper finally argues for the need of a rational discourse among chemists on the aims of chemistry.

1. Introduction: The exponential growth of chemistry

Looking retrospectively at chemistry at the end of the 20th century, we use to emphasize the great achievements of the century. In that regard, the record of Nobel prizes nicely provides us with one highlight per year. However, without diminishing these honorable achievements, such a retrospective view needs correction in two regards. First, a single achievement can by no means be representative of several hundred thousand other achievements made in the same year. And secondly, it gives the impression that science would grow linearly, with a constant number of achievements per year. Instead, science grows exponentially with doubling times of 12-15 years (Price, 1961). Only during the past 15 years we saw more chemistry publications than had been written ever before (CAS, 1998). And this year chemists will publish a hundred times as many papers than in 1901, when van't Hoff received the first chemistry Nobel prize.

The focus of the present paper is not on so-called highlights of chemistry, but on ordinary or average chemistry, so to speak. Only if we put aside our favorite subjects of chemistry and regard what all the millions of chemists worldwide are doing, we have a chance to get some more objective insight in what happens in chemistry as a whole. As a philosopher trained in chemistry my general interest is in philosophical issue of chemistry (e.g. Schummer, 1997a). But, surprisingly, chemistry seems to evade all kinds of received philosophical approaches, such that philosophers of science simply neglected chemistry until recently. Even today many philosophers think that quantum chemistry and its relation to quantum mechanics is the only issue worthwhile thinking about. Chemistry proper appears to be something that does not fit our received image of science. In fact, the most striking feature of chemistry is that it does not simply describe and explain our world as it is; chemists rather produce their own objects of investigations, *i.e.* they make new chemical substances.

The making of new substances is by no means a *marginalia*. In quantitative terms it is by far the main activity of chemists. A sample survey of 400 papers on 'general chemistry' has shown that some 75% present at least one new substance (Schummer, 1997c). On the average, every paper abstracted by Chemical Abstracts today presents 2 new substances. We even have much evidence that the making of new substances has constantly been the main activity of chemists during the past 200 years (Schummer, 1997b). The number of known substances has been growing exponentially since 1800, from some hundreds then to about 19 million today. Since the number constantly doubles every 13 years during the whole period, it is not a bad estimate saying that we will have nearly 80 million substances in 2025, and about 300 million in 2050. If the next century will show the same growth rate as the two previous centuries did, we should expect to deal with nearly 5 billion substances in 2100!

In what follows, I am going to discuss some problems arising from the exponential growth of substances and the corresponding knowledge. First of all I regard how the documentation and education of chemistry can cope with that development. Then I throw a philosophical glance at the growth of chemical knowledge and compare it with our lack of chemical knowledge. Finally I address the blind spot, why chemists are making new substances at all. After regarding how chemists implicitly answer that question, I argue for an explicit and rational discourse about the aims of chemistry.

2. Challenges for chemistry documentation and education

2.1 Chemistry documentation and the principle of completeness

Science documentation systems, such as libraries, abstract journals, citation indices, bibliographies, handbooks, source databases *etc.*, are directed by the *principle of completeness* with regard to their respective sort of information. First of all, every information unit is of the same value, as long as it belongs to the field and is reliable according to standards of scientific method. A kind of information hierarchy is introduced only implicitly because of requirements of finding and retrieving information. For instance, a subject or a keyword index covers only items considered to be 'important'. And the division of a scientific field into sections and subsections reflects in some way the state of the corresponding research fields; occasionally it needs adjustment, if new research fields emerge or if formerly 'unimportant' fields are getting more 'important', and *vice versa*. But in general, the principle of completeness is inconsistent with any kind of selectivity. In particular, it requires that we must strictly ignore utility criteria based on our current needs. We must not ask what a certain information is good for. It might be that it becomes important in the far future to solve problems of which we have not yet the slightest idea today. The mere possibility is sufficient to justify documentation.

It goes without saying that the principle of completeness seriously challenges all individuals and institutions concerned with the rapidly growing information in fields such as chemistry. Chemistry is by far the most productive science, if we consider the number of papers abstracted by *Chemical Abstracts*. Chemists produce even more papers than all other natural and social sciences together (Tague *et al.,* 1981). To be up-to-date in all areas of chemistry you would currently have to read about 2,000 new publications every day (CAS, 1998). If you prefer to screen only the short abstracts, you must read 200 pages per day or about 70,000 pages per year. Furthermore, since the number of chemistry publications increases also exponentially, you need to double your reading capacity within the next 15 years.

The most significant challenge for institutions is to cope with economic limitations. According to all scientometric measures (number of scientists, publications, journals *etc.*) science, and in particular chemistry, have been growing much faster during the past hundred years than, for instance, the world product and the world population. An ideal documentation system would make available all information to all chemists. Primary chemical information is for the most part published in journals of which Chemical Abstracts currently monitors over 8,000. Based on the number of authors of publications abstracted by CA, there are currently about 3 million chemists worldwide. According to a rough estimate the ideal documentation system of chemistry would cost several hundred billion dollars each year only for subscription, let alone the costs for storekeeping and information processing, which might be considerably reduced by electronic publishing.

Of course, nobody is capable to read all publications of chemistry, not even all publications of a small area. Thus, being up-to-date, being universally informed and competent has become a mere fiction since many decades. And of course no common science library, except a handful of mega-libraries, is capable to subscribe to all chemistry journals. The immense production of chemistry information has considerably changed the whole system.

First of all, primary sources of information, *i.e.* chemistry journals, have lost their former significance in favor of secondary sources, *i.e.* searchable databases. Beside a few leading journals in each area, which attract readers mainly by review articles, the vast majority of chemistry journals are noticed today only indirectly through the filter of databases. To be sure, secondary sources have a longstanding tradition in chemistry in the form of handbooks, most notable the handbooks of Gmelin (since 1817) and Beilstein (since 1880). But the role of secondary sources has gradually changed. Formerly mainly intended to provide surveys and references, secondary sources have today become the proper information source in the form of electronic databases. That is how chemistry documentation systems have responded to the mentioned challenges. Professional paper analysis together with fast electronic information processing and retrieving have provided a new information level that tries to meet the requirements both of completeness and accessibility to up-to-date information.

Let us regard some consequences of the changing situation. First, there are new demands both on the documentation system and its users. Paper analysis and information processing is no mere information collection but a kind of text interpretation that violates the principle of completeness per definition. We necessarily need criteria to decide what should count as significant information to be fed into the database. The demand on the 'information manager' would ideally be to foresee all kinds of questions that people might put in the far future. Because the focus of scientific interest naturally changes in the course of time, it is impossible to meet that requirement. Consequently, lots of information of the primary sources, which may become significant in the future, will be not retrievable from the database. Switching from browsing to searching makes a substantial difference in information access for users. If you want to search a database, you are expected to know before, what you are looking for, and you need to know that even in exact terms of the search system. Moreover, there are kinds of scientific problems, in particular in innovative research areas, which cannot be formulated in terms of clear-cut question or keywords, and for which browsing would be the more appropriate kind of access.

Secondly, the changing situation has also impact both on the style of writing and the kind of information presented in journal papers. Formerly authors addressed their papers first of all to colleagues of their scientific community (so-called 'communications'). Today papers are more and more addressed to information managers whose task is to extract the relevant information to be fed into a database. Thus, the style has become rather technical and schematical; authors try hard to make all information as explicit as possible. Moreover, if the aim of a paper is to contribute to a database, the presented information is also supposed to be tailored to the categories of the database. Thus we hardly find speculations, hypotheses or any other more complex form of reasoning in chemical papers. Instead, the vast majority of chemistry papers are centered on new substances, its preparation and properties, including structure and reactivity (Schummer, 1997c). Today, every paper abstracted by Chemical Abstracts presents 2 new substances, on the average, compared with about 0.5 in 1950 (Schummer, 1997b, p. 118)! Since chemical substances form the major category to systematize chemical information in databases, this trend seems to be no pure chance. Instead we have evidence to believe, that the documentation system has indirect impact on the kind of information produced by chemists. In other words, chemists' inclination to proliferate the number of substances is not only documented; the documentation system is supposed to have also influence on chemists' inclination to make more new substances.

2.2 Chemistry education and principles of selectivity

The documentation system and the education system are first of all similar in their knowledge orientation toward the future. Information is documented because of its possible usefulness in the future. And young people are educated in chemistry because we believe that they will need chemical knowledge in the future. However both systems must deal with the growth of knowledge exactly the opposite. While documentation systems try to apply the principle of completeness, educational systems are forced to apply reasonable *principles of selectivity*. The need of selectivity necessarily follows from the limited time resources for chemistry education. In my view, a main debate in professional chemistry education is centered on the question: What kind of selectivity principle shall we reasonably apply to extract those parts of chemical knowledge to be taught at school, high school, and university level, respectively?

A first answer can be derived from the last section; namely that a certain concept of selection does not make sense any longer. As we have pointed out, *nobody can actually have an overview of the whole of chemical knowledge*. It is definitely impossible for human beings. Remember that you must read 20 publications every day in order to grasp only 1% of the overall chemical publications! However, in order to make a selection, you must first of all know the whole. If reading 20 publications a day is something of an upper limit, we can follow that whatever chemistry authorities claim, their scope of knowledge of primary sources is at best 1%. As a consequence, every selection of chemical knowledge by human beings is necessarily arbitrary.

As we have seen, the chemical documentation system tries to cope with the proliferating mass of chemical knowledge by feeding databases with searchable information. Thus, the only way to select parts from the whole of chemical knowledge is to use the search function of databases. But that is not the kind of selection chemistry education is in need of, since we cannot search databases according to criteria of significance.

The lack of reflection on this issue has led chemistry teaching, at least at the university level, into absurd situations. Some 150 years ago chemistry handbooks were written to fulfil also the needs of chemistry education, *i.e.* there was no difference between *handbooks* and *textbooks* at the university level. The necessity of textbooks as an own genre came from the immense growth of the extent of handbooks. Thus a chemistry textbook was composed of like a digest of a handbook, *i.e.* a structured collection of facts. Even though the past 20 years have provided some new and excellent accounts of chemistry textbook writing, there is still a prevailing tendency in chemistry to write textbooks as digests of handbooks. The absurdity of this textbook tradition gets clear, if we consider the growth of information for handbooks, nowadays stored in databases. Since we have doubling times of about 12-15 years during the whole period, the amount of 'handbook information' is now over 1,000 times the amount of 150 years ago! Given the impossibility of an overview, as pointed out above, these textbooks present no longer something of a digest, but an entirely arbitrary selection of information. Such a selection is in the strict sense arbitrary, because nobody can give any objective reasons to justify the selection. If these textbooks are used as the basis of chemistry courses – and they are still used at the university level –, then we must conclude that the underlying teaching concept is a fundamental confusion: students are confused with databases, to be fed with an arbitrary selection of chemical information.

If we do not confuse students with databases but consider them possible users of databases, it follows that *students should learn how to retrieve and use information from databases*. Using a telephone does not require learning a phone book by heart, but a lot of other general abilities. Similarly, using a chemical database requires a great deal of chemical knowledge, quite different from the kind of knowledge stored in a database. We must know what kind of information is stored in what kind of database, and what is not stored at all. We must know what kind of information might be useful to solve a certain problem, and how it can be transformed or adapted to our problem. We must know, how to find the information in the database, *i.e.* how to use the search categories. And last but not least we must know, what is a problem at all that could be solved by using a chemical database.

I can not go into details here, but I like to stress only two general points. First, the shift from learning database data to learning database rules implies a reasonable selectivity principle to cope with the growth of information. For the ability to use a database is relatively independent of the amount of information stored in the database. Secondly, the shift also implies different emphasis on chemical knowledge. Databases provide answers to certain questions; *i.e.* the use of database is basically a *problem approach*. Instead of learning answers to possible questions, students must learn to put questions to which they might find possible answers. Hence the emphasis is on problems. It is important to note that these problems need not be internal problems of chemistry. While the answers are definitely chemical, the problems may also come from quite different areas, from neighboring disciplines, from politics, from ordinary life, etc. Thus, *chemical competence necessarily transcends the scope of chemistry proper*.

As I said above, young people are educated in chemistry because we believe that they will need chemical knowledge in the future. Since we currently know neither the problems of the future nor the appropriate knowledge to solve these problems, it follows that students should first of all be trained in two regards. They should become able to recognize problems that can be tackled with chemical knowledge, and they must be able to collect the relevant knowledge on their own.

3. Philosophical valuation of the growth of chemical knowledge

3.1 Philosophical optimism versus pessimism

Today philosophers of science can roughly be divided up concerning their view on an absolute growth of scientific knowledge. Traditionally, most philosophers held an optimistic view claiming that scientific progress based on an absolute growth of knowledge is possible. Kuhn, Feyerabend, and others seriously criticized that view in the 1960s through historical and methodological arguments. (A classic reader on the debate is Lakatos/Musgrave 1970.) Both groups share the common assumption that scientific knowledge is somehow stored in theories (instead of databases). The skeptic or pessimistic view says that a change of theories, or a change of paradigms in the Kuhnean sense, may be regarded as a radical break of the scientific development, making the states of science before and after the break incommensurable with each other. Incommensurability means, that we cannot compare the two states and, consequently, that we cannot claim that the change is a progress or regress of science. Optimists, first of all Popper and his followers, denied the incommensurability thesis. They suggested that a change of theories should be accompanied by some kind of improvement according to absolute criteria. While theories are always subject to possible falsification, Popper optimistically claimed that the scientific development would come, step by step, closer to truth (*verisimilitude*).

Let us regard now, if our results on the exponential growth of chemical substances may contribute to that philosophical debate. Obviously new substances are not new theories. Nonetheless, chemists characterize every new substance through various material properties. Hence, with every new substance our chemical knowledge is extended by a certain amount of information. It is hard imagine how this kind of chemical knowledge could be affected by a change of theories. At least the knowledge how to produce the new substance seems to be entirely resistant to any kind of theory change. As a consequence, there is cumulative growth of chemical knowledge along with the production and characterization of new substances. Furthermore, we can roughly estimate the growth of knowledge in quantitative terms. Since every new substance is characterized at least by some basic material properties, exponential growth of substances goes along with at least exponential growth of chemical knowledge. That is to say that the skeptical view on the growth of knowledge does not generally stand up if we regard chemistry.

Are we then obliged to hold the optimistic view? First we should note that philosophers' persistent neglect of chemistry has led to the situation that is it rather difficult to apply their concepts to chemistry at all. The idea of a universal theory (or a sequence of succeeding theories towards a perfect description of our world) may be justifiable when dealing with theoretical physics. But we hardly find any correspondence in other scientific disciplines including chemistry. Not only are chemical theories for the most part restricted or tailored to a certain scope of phenomena or a certain realm of substances. Chemists are also permanently *changing* the world, of which philosophers think that it would only be described and explained by scientists. Referring to concepts such as truth or verisimilitude of theories, philosophers like Popper seem to presuppose a given, fixed, and finite world. However, one of the main activities of chemists is, as we have seen above, the making of new substances, *i.e.* changing and extending our world.

If we take that into account, we must evaluate the growth of chemical knowledge from quite a different perspective. There are at least two reasons that lead us to a less optimistic evaluation.

3.2 The growth of knowledge in the face of an infinity of possible knowledge

We have no reason at all to assume that the realm of possible substances is limited. If we take that seriously, we must assess the finite growth of chemical knowledge against the background of an *infinity of possible knowledge*. An infinite realm of possible substances corresponds to an infinite amount of possible knowledge that we not yet have. To be sure, the fast increase of our chemical knowledge decreases our lack of knowledge in a certain sense. But that does not matter. Mathematics forces us to accept that a finite decrease of an infinite amount does not affect the infinity at all. As a consequence, whatever the rates of growth of chemical knowledge will be, that does not change the fact that *our knowledge gap is infinite and will remain infinite in the future*.

Chemists are not used to reflect on the infinity of possible knowledge. And many may think that it is just playing about. Surely, whether the realm of possible knowledge is infinite or not, does not directly affect the research of an individual chemist. However it has far-reaching consequences concerning the entire enterprise of the chemical science, and as such it indirectly affects the research of an individual. Against the background of an infinity of possible knowledge, completeness of knowledge cannot be a goal in chemistry, in contrast to other sciences such as botany, zoology or even physics. Against the background of an infinity of possible research, the decision for one or the other research field cannot be justified by traditional epistemological reasons, *e.g.* understanding the world as it is. Against the background of an infinity of possible substances, the making of new substances gains some arbitrariness: why producing these substances and not others? Sciences faced with the infinity of possible knowledge call for other reasons than traditional epistemological reasons; the mere quantitative growth of knowledge is no longer a sufficient justification.

In sum, even though we definitely have exponential growth of knowledge in chemistry, that does not suffice to share the optimistic view of some philosophers. Instead, in the face of an infinity of possible knowledge, the growth of actual knowledge calls for evaluation based on values different from traditional epistemological values.

3.3 The growth of chemical knowledge increases our lack of knowledge

There is a second, perhaps more important, reason to refute any optimistic view on the growth of chemical knowledge: The exponential proliferation of new substances goes along with overexponential proliferation of further *possible* chemical knowledge, *i.e. new chemical knowledge even increases our chemical 'nonknowledge'*. What seems to be a paradox, is actually a peculiarity of chemical properties. Chemical properties tell us something about the reactivity of two or more substances to form other substances. Thus the number of possible chemical properties depends on the number of combinations of already existing substances. The more substances we have, the greater the number of combinations of substances for possible reactions. If our world consists of *n* substances, then the production of a single new substance allows considering *n* new pair combinations of substances, *i.e. n* new possible reaction pairs. If we regard also reaction triplets, quadruplets, *etc.* as well as variations of concentrations and other reaction condition, the number of new possible chemical properties grows immensely. It is not necessary, that every combination actually leads to chemical reaction. What counts is the mere possibility, *i.e.* our lack of knowledge in advance.

Let us regard now, how this philosophical reflection might concern chemistry and the society. The growth of our lack of knowledge is both a chance and a risk. First, every new substance makes us aware of new knowledge gaps and as such it may guide chemical research. Every new substance opens up a wealth of new possible chemical reactions. Thus it immensely increases the capacity for making further new substances. In other words, new substances serve to make further new substances. In fact, there is some evidence that this kind of 'feedback' is actually responsible for the *exponential* growth of substances in some areas (Schummer, 1997b/c). The growing lack of knowledge is a kind of driving force for chemical research. Of course the overall knowledge gap increases much faster than our overall knowledge, as shown above. But the case is different in delimited fields, where a few so-called 'key substances' may open up the chemistry of entire substance classes.

If we leave the laboratory and, in particular, if our new substances leave the laboratory, the growth of our knowledge gap is getting a serious problem that we are all concerned with. In the laboratory, chemical reactivity studies deal with very simple chemical systems, mainly with pairs or triplets of selected pure substances. Whatever the guiding selection rules are, we know that laboratory research can grasp only a diminutive and diminishing fraction of the whole of chemical properties. Real or 'natural' systems, on the other hand, are terribly complex and do not care about laboratory selections. Real systems should be expected to reveal the whole complexity of chemical properties. Thus real systems confront us with our actual epistemological situation, namely a rapid growth of our lack of knowledge. Our simplistic mathematical reasoning gets important now: If our world consists of n substances, the addition of a single new substance allows to consider n new possible reaction pairs to form new chemical products, which may be subject to further reaction, and so on. From the chemical point of view, our world is not a mere collection of substances, but a complex dynamic reaction system. The addition of only one new substance can effect an uncountable number of unforeseeable changes. And all we know, the addition of two substances does not merely double the number of unforeseeable changes. Taking that into account, the current exponential growth of new substances – not only in the laboratory, but also in our environment – finally leads us to a rather pessimistic evaluation of chemical knowledge. We are forced to admit that, due to chemical changes of our material environment, the chemical understanding of the same material environment is losing ground much more rapidly. (To avoid possible misunderstandings, I should emphasize that I do not wish to conjure up something like an environmental catastrophe. In contrast, my thesis is that we rapidly decrease chemical knowledge about our future environment.)

4. The aims of chemistry

From the point of view of philosophy of science, it is extremely difficult to understand what chemistry is all about. That is partly due to the one-sided concepts of science philosophers have been propagating during the past centuries. They simply confused a small area of physics with the whole of science or, to be more correct, with the wealth of scientific disciplines. Understanding the world as it is in terms of universal theories is certainly an honorable objective. But it is definitely not the only one in sciences, and for many fields it does not even make sense. For instance, the making of new substances – a central activity of chemists during the past 200 years, as we have seen –, does not describe but change the world; and thus it is even counter-productive to the understanding of the given world. In the received view, that activity would not be science at all. However, despite the one-sided focus of traditional philosophy of science, its general approach is useful, namely understanding sciences in terms of their aims and methods. *The main difficulties in understanding chemistry arise from the fact that we (non-chemists as well as chemists!) have no clear idea about the aims of chemistry.* It is even my personal impression that chemists try hard to avoid this question.

Before we discuss the issue, it is first of all necessary to point out the difference between psychological motives of an individual scientist and the aims of a scientific discipline. Individual scientists pursue happiness, satisfaction of curiosity, reputation, honor, power, money, *etc.*, depending on their personal values. A scientific discipline, on the other hand, establishes values on quite a different level and of different types, some of them discussed by philosophers of professional ethics. Unlike psychological motives, the aims of scientific disciplines are manifested in more or less implicit community rules for the valuation of scientific activities. Let us confine ourselves to the valuation of scientific results. Results are measured according to what extend they contribute to achieving the aims of the scientific discipline. Thus, in terms of classical philosophy of science, a result would be worthless if it does not contribute to our understanding of the given world, despite the personal satisfaction the individual researcher may have.

As I said already, 'understanding the world as it is' can definitely not be the aim of making new substances. What then are the scientific aims of this central chemical activity? Why do chemists make new substances? Are there scientific aims at all, and how could we grasp them?

4.1 Implicit aims of making new substances

There is no explicit discourse about the general scientific aims of making new substances in chemistry. Of course every chemist is able to give some reasons in terms of his or her particular subfield. But such reasons are for the most part incomprehensible by people outside the subfield, because the reasons refer to specific values comprehensible and accepted only by members of the corresponding subcommunity. In contrast, general scientific aims of chemistry are based on values comprehensible and accepted by the majority of chemists. Since there is no explicit discourse on general aims in chemistry, we must look for instances where values are at least implicitly at work. Such is the case, where chemical results are measured according to the significance for a general chemistry readership. In fact, journals on general chemistry demand from authors to point out the general significance of their results in general terms. Thus the reasons given by authors on demand implicitly reflect the scientific values accepted by the chemical community. Note that the reasons need not correspond to psychological motives, but they must refer in some way to generally accepted values. Therefore, papers in journals of general chemistry are a valuable source to grasp the values and aims of making new substances. The following results are based on a careful text analysis of 300 papers published between 1980 and 1995 in the *Angewandte Chemie* (Schummer, 1997c). Every paper presented at least one new substance as well as reasons for the general significance of the results.

A widespread misconception is that the making of new substances as such is an entirely technological enterprise. However, as I have pointed out elsewhere (Schummer, 1997d), all received concepts to distinguish between science and technology fail, if we try to apply them to chemistry, because they depend on either one-sided, outdated, or arbitrary concepts of science. Nonetheless, possible application of new substances is an accepted aim in the chemical community. However, if we regard the reasons for making new substances, as presented by chemists in their publications, it turns out that about 77 % do not consider at all possible technological applications of their substances – we do not even find briefest mention. To be sure, technological application has become a significant justification to raise research funds. Thus, there is some increase of mentioning possible applications of new substances during the past 15 years. But that is only a rhetorical shift. The truth is that the number of substances grows much faster than the number of chemistry patents, which is a good measure for applied research. On the average, chemists today produce twice as many substances per patent than in 1980 (CAS, 1998). Hence, application plays only a minor and even decreasing role in the making of new substances – despite the fact that many chemists think it would be the main goal (*e.g.* Pimentel *et al.,* 1985).

I emphasize once again, *the making of new substances is by far the largest scientific endeavor of all sciences today*. Since its guiding aim is neither understanding the world as it is nor technological application, the whole wisdom of received philosophy of science does not help much to understand the largest scientific endeavor!

Also neo-positivistic philosophy of science give us not much insight in the chemical activity. To be sure, the making of new substances is basically a kind of experimental activity. But only in exceptional cases (about 8%) it serves to test or modify some kind of theories or laws. In other words, whatever philosophers of science have said about falsification, verification, and exhausting of scientific theories in this century, it is not very significant in chemistry.

When chemists are required to point out the general significance of their results, they tend to emphasize either the *novelty* or the *unusualness* of their products. In many cases the use of terms like 'new' and 'unusual' simply reflects the embarrassing situation of chemists, when forced to talk about aims and values of their research in general terms. But beside these rhetoric uses of 'new' and 'unusual', it is frequently possible to recognize scientific values.

Since the novelty of a new substance is self-evident, chemists lay stress on the fact that the new substance is an exemplar of a new substance class, or at least an 'considerably enrichment' of a still less known substance class. Thus, the *extension and enrichment of the chemical substance classification* seems to be an accepted scientific aim in chemistry. About 13% of papers in preparative chemistry refer to it, in inorganic chemistry it is even 25%.

The use of the terms 'unusual' or 'extraordinary' by chemists is more difficult to understand, because it presupposes concepts of 'usual' or 'ordinary' that remain for the most part implicit, sometimes even obscure. In most cases 'unusual' is related to structural properties of the nuclear framework (such as bond length and angle, coordination number, symmetry), or to the electron structure (type of bonding, charge distribution, conjugation, mobility, *etc.*). In none of the analyzed papers 'unusual' means 'inconsistent with our theories'. Instead the underlying concepts of 'usual' rather refer to some sort of structure typology, simplistic approach, rule of thumb, or familiarity, which chemists used to cope with the diversity of phenomena. Whatever it is, chemists undoubtedly have a considerable fable for structural features. About 11% of the papers of preparative chemistry (18% of inorganic chemistry) justify their making of new substances by referring to structural features of their products. Hence, we should regard the *search for structural feature as an accepted scientific aim of chemistry*.

Readers who have counted the percentage numbers mentioned above will be missing another 45%. What else could be a reason for making new substances? The most surprising result of the paper analysis is that the great majority of preparative chemists (45%, in organic chemistry even 53%) make new substances to further improve the synthetic capacities of chemistry: The new substance is expected to serve as useful reagent or catalyst. The specific way of making a new substance is offered as a general method to make plenty of other new substances. New substances spill out of chemical reaction studies aiming at theoretical guides for chemical synthesis, *etc.* In other words, the main reason for preparing new substances is the improvement of synthetic capacities. That is to say that *the making of new substances is actually an end in itself in chemistry*.

There is much evidence that the making of new substances as an end in itself has persistently been the central scientific aim of preparative chemistry during the past 150 years. In fact it is the only reasonable explanation for the stable exponential growth of substances during that period (Schummer, 1997b/c). Only if the synthetic capacity constantly grows along with the number of substances, exponential growth of substances is possible.

4.2 The need for a rational discourse on the aims of chemistry

While there is no explicit discourse on aims in chemistry, aims are nonetheless implicitly at work, as the previous section has shown. The general difference between implicit and explicit aims is that only the latter are subject to rational argumentation, justification as well as criticism. Implicit aims of a community are for the most part unconscious aims, historically inscribed on the organizational structure of the community. Implicit aims, and their corresponding values, may be more effective in guiding the community, since there is no critical discourse about directives. However, implicit aims may lead toward situations that nobody wants. Making aims and values explicit and subject to rational discourse was the central idea of enlightenment and modernity. As far as we know, that is still the best way to suit the aims of a community with the preferences of its members. And at the same time it places the responsibility for any development on the members of the community. Let me finally give some reasons, why an explicit discourse about aims in chemistry is in need.

Autonomy: Implicit aims may be subject to implicit changes by external impacts. Since they are inscribed on the organizational structure of the community, a change of the organizational structure may directly cause a change of the aims. Thus, a science without an explicit discourse on its aims is at the mercy of external impacts and aims; *i.e.* it has no autonomy.

Among external impacts, the distribution of research funds is certainly the most powerful one that is even increasing with the costs of research. Distribution of funds is at best governed by the prospective needs of the society. While the actual needs of the society are subject to change, our opinions about the prospective needs are even more and controversial too. I do not want to argue that science should not consider the needs of the society. In contrast, I even hold it very important. However, a science that does not define its own aims and methods, *i.e.* its own identity, is a plaything of changing and opposing foreign opinions that would not be very helpful here.

Comprehensibility: An explicit discourse on the aims of chemistry would help understand this science better. As I said already, the lack of clear ideas about the aims of chemistry is the main obstacle for nonchemists, for becoming chemists, and for chemists. To start with nonchemists: Not only would philosophers of science become able to correct their one-sided concept of science. Also the public image of chemistry could lose its fancifulness, its associations with demonic powers, which have filled the gap of understanding chemistry since many centuries.

Understanding chemistry in terms of its aims and their corresponding values is a key to chemistry education. Only if we are able to tell students what chemistry is all about, they get at all qualified to decide, whether they are interested in chemistry or not. For to be interested in a science means that one is able to relate the aims and values of that science to one's own personal values. Furthermore, understanding chemistry in terms of its aims and values enables us to develop reasonable principles of selectivity. Despite the shift suggested in Sect. 2.2, principles of selectivity are still in need for organizing chemistry courses, for writing introductory as well as advanced chemistry textbooks, *etc*. Every reasonable selection presupposes values to decide what is more important and what is less.

Finally, also working chemists can profit much from an explicit discourse on the aims of chemistry. Not only does it make the standards of research valuation more transparent; research is also more efficient in the face of a clear idea about its aims. Moreover, participating in a rational discourse on aims is part of the academic tradition in the proper sense. It requires quite different intellectual qualifications than research proper, and as such it is a central enrichment of intellectual life. Scholars need to be engaged both in research and public reflection on research in order to avoid alienation and heteronomy – two archenemies of scientific creativity.

Let me conclude with some final remarks, how a rational discourse on the aims of chemistry might critically address the most important implicit aim of chemistry, namely the proliferation of chemical substances. In general, activities having an end in themselves are indispensable, since they define at all the values according to which all other activities are to be measured. But there is some doubt, that the proliferation of substances is a reasonable choice in this regard.

First, we should analyze in more detail, to what extend the proliferation of substance is indirectly governed by the specific kind of chemistry documentation. As pointed out in Sect. 2.1, chemical substances form the major category to systematize chemical knowledge. To make an obviously new contribution to the scope of chemical knowledge, chemists may feel obliged to connect their result with a new substance. If that were actually the case, there would be a strange inversion of priorities. Instead of a documentation system being governed by the aims of science, research would be governed by the requirements of the documentation system.

Secondly, since chemistry is not only a practical but also a cognitive enterprise, we may ask how the proliferation of substances contributes to the scope of knowledge compared with the scope of 'nonknowledge'. A discourse on the aims of chemistry is in particular challenged by the problems pointed out in Sect. 3, namely that the proliferation of substances does not decrease but increase the infinite scope of 'nonknowledge'.

It is not the task of a philosopher to prescribe aims and values to the chemical community. We may only analyze what kind of implicit aims are at work, point out general reasons for making aims explicit, and give assistance to a rational discourse. Eventually it is up to the members of the chemical community to start a rational discourse about their aims.

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