Jointly published by Elsevier Science Ltd, Oxford
and Akadémiai Kiadó, Budapest

Scientometrics,
Vol. 39, No. 1 (1997) 125–140

SCIENTOMETRIC STUDIES ON CHEMISTRY II: AIMS AND METHODS OF PRODUCING NEW CHEMICAL SUBSTANCES

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(Received January 20, 1997)

Chemistry, as today's most active science, has increased its substances exponentially during the past 200 years without saturation. To get more insight why and how chemists produce new substances, a content analysis of 300 communications to the *Angewandte Chemie* of the years 1980, 1990, and 1995 is carried out regarding aims and methods of preparative research. In the most productive field of organic chemistry production mainly occurs to improve abilities for further production, while the less productive field of inorganic chemistry has more diverse aims. Methodological differences between organic and inorganic chemistry are discussed in detail as well as the relationship between pure and applied science.

1. Introduction

Chemistry is by far today's most active science with regard to bibliometrical indicators. In part I of my scientometric studies on chemistry,[1] I have pointed out that producing new chemical substances is a central activity of this science. There is a rapid exponential growth of chemical substances during the past 200 years (doubling time of 12.9 years) without saturation until today. It was argued that, since pure external explanations are implausible, the growth of chemical substances is to be explained by internal or methodological approaches. Such a methodological approach should also consider the different productivity of organic and inorganic chemistry, that makes more than 95% of today's known substances to belong to organic chemistry.

The present study tries to understand the research process in terms of aims and methods of preparative organic and inorganic chemistry. It is based on content analysis of 300 papers of the *Angewandte Chemie* that is one of the most important international chemical periodicals today. If we assume that there are no fundamental changes of the internal research process during periods of stable growth, then an investigation on

0138–9130/97/US $ 15.00
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recent preparative chemistry might give some insight in the process of the last stable period.

Methodological investigations carried out with statistical means run the risk of falling between two stools. Methodology, on the one hand, is the domain of philosophers of science. Their concern is traditionally the pursuit of truth that is dealt with either on rationalistic grounds or on the basis of single historical case studies. Statistical investigations on science, on the other hand, is the domain of scientometrics that seems to be rather restrained in dealing with methodological questions hitherto. While chemistry has been nearly neglected by philosophers of science,[2] it is one of the earliest and most frequent topics of bibliometric studies, not least because of the exemplary documentation system *of Chemical Abstracts.*[3] This study is based on optimism that some philosophical (methodological) questions may also be tackled by scientometric methods to provide a more sophisticated empirical picture of our sciences.

2. General characteristics of the text corpus

2.1. Characteristics and topics of the Angewandte Chemie

The *Angewandte Chemie* is one of the leading international journals of chemistry with regard to the ISI journal impact factor.[4] There are 12 issues (since 1995: 22 issues) a year each in a German and (since 1961 also) in an international edition addressed to a general readership of chemists. Besides two or three extended *Essays* on actual topics of any field of chemistry, some *Book Reviews,* and (since 1994) so-called *Highlights* (short reviews on recent topics), each issue contains 20–30 *Communications* ("Zuschriften"). Since 1975 a stable set of *Instructions for Authors* is regulating the *communications* as short communications (max. 6 typewritten text pages) on preliminary or final results of any field of chemistry. Authors are urged to submit results only of "general interest" with respect to "significance, novelty or wide application" that must be discernible by non-specialists. They are further requested to give explicit reasons within the text for an urgent publication in this sense. The *Instructions for Authors* ensure that communications since the late 1970s can be considered as a uniform text sort with constant pressure to justify chemical research within a general context.

With regard to the sections of *Chemical Abstracts,* communications to the *Angewandte Chemie* reveal a clear-cut thematic profile.[5] Besides classic fields of organic and inorganic chemistry the major part is on metall-organic chemistry;

biochemistry, polymer chemistry, applied chemistry, chemical technology, general physical and theoretical chemistry are hardly represented. Moreover, there is an obvious preference for preparative research. A survey of the years 1980, 1990, and 1995 reveals that throughout about 75% of the communications mainly report on the production and characterization of at least one new chemical substance. Of them more than 90% are from institutes of organic or inorganic chemistry in equal parts. Compared with an average paper refered by *Chemical Abstracts*[6] the number of new substances per communications of the *Angewandte Chemie* is 2–3 times higher. Hence, the journal provides a source for outstanding preparative research on classic organic, inorganic and metall-organic chemistry.

2.2. *Selected papers and general trends*

For the present study, random selections of 100 communications of the *Angewandte Chemie* each of the years 1980, 1990, and 1995 were made in which the production and characterization of at least one new substance are a central part. Besides the main study on aims and methods of preparative research, additional data were collected to consider possibly significant trends: nationality, academic status, institutional origin, sex, number of authors, number of reported new substance (Table 1).

During the period under investigation the most obvious trend is towards internationalization of authors in two steps.[7] Prior to 1980 the great majority of authors were still Germans; a first change was in favour of other European authors in the 1980s and a second change in favour of North American authors in the early 1990s.[8]

Several indicators suggest that research and publication standards have been considerably raised since 1980. The acception rate declines dramatically, although the number of published communications has been nearly doubled.[9] Both the number of authors on average and the maximum academic status has been increased.[10] At the same time the number of new substances per paper goes through a minimum. These trends can be partly explained by a raise of analytical standards to characterize new substances. The increase of pages per paper is mainly due to analytical data presented in figures and tables. Laboratories with specialized equipment are urged to co-operate with each other, while co-operation is ordinarily arranged by leaders of research groups (professors).[11]

Table 1
Trend statistics of communications of the *Angewandte Chemie*

	Year 1980	1990	1995
1. General statistics			
number of comm. selected/total	100/325	100/340	100/510
preparative comm. (%)	73	76	76
pages per comm.	1.22	1.85	2.5
acception rate (%)	75–80	50	48
2. Author statistics (selected comm. only)			
number of authors per comm.	3.0	3.6	4.1
female authors (%)	6	9	11
comm. with at least 1 author of professor status (%)	78	81	88
national origin of correspondent author			
Germany	81	64	49
other European countries	7	24	23
North America	7	10	23
all others	5	2	5
institutional origin of correspondent author			
inorganic chemistry	44	42	37
organic & biochemistry	47	40	47
physical chemistry	2	0	0
technol. & polymer chemistry	2	6	6
industry	1	2	2
uncertain	4	10	8
3. Productivity statistics			
New substances per selected comm.			
total	4.7	3.9	4.5
inorganic chemistry	3.1	2.7	3.4
organic & biochemistry	6.3	5.6	5.9

3. Methods

3.1. Determining the aims of preparative chemistry

Production and characterization of at least one new chemical substance is a central part of all considered communications. According to the editor's instructions, authors are urged to give explicit reasons, why their preparative results are of general interest (Sect. 2.1). Hence, extracting these reasons from the communications should provide a survey of aims in preparative chemistry.

Certainly, there are discrepancies between the reasons given in the text and the author's actual research motives in some cases. Personal motives or even a lack of research motives (in cases of results by chance) may be covered by ex-post reasoning. But our interest is not in psychological analysis of researchers' motives. Instead we may suppose that a given reason on demand of the editor is always an accepted reason by the scientific community, and that the given reasons as a whole approximately represent the aims of the community of preparative chemists, both with regard to kind and weight.[12]

To extract the reasons from the papers systematically, a sophisticated scheme of aims of chemical research was developed, which is presented in the following (condensed) form:

(1) Theory: According to mainstream philosophy of science, scientific experiments are performed to test, develop or modify theoretical concepts. Theoretical concepts in a broader sense are general theories, models, rules, and analogies.[13] Theory relevance is indicated, if authors compare empirical and theoretical results in order to test or improve theoretical concepts. Recommending a new substance as a model for further theoretical investigation is also considered to be theory relevant.

(2) Classification: Unlike physics, chemistry has always been concerned with classificatory problems. Preparative research is considered to be of classification relevance, if authors emphasize that the new substance is a prototype or an important expansion of a substance class. Further cases are undermining established classificatory lines by the new substance or proving the existence of a substance that has been doubted hitherto.

(3) Synthesis: Since the increase of substances is a main characteristic of chemistry, the improvement of preparative methods is also likely to be an important aim of preparative research. Synthesis relevance is registered, (a) if the new substance is recommended for further synthesis (as starting substance, reagent, catalyst etc.), (b) if the new substance is exemplarily produced by a new method which is recommended for further analogy preparation or (c) if the new substance is gained as a side-product in the course of developing a new reaction mechanism by chemical methods in order to enlarge preparative methods on theoretical level. Synthesis relevance is also registered, if the new substance was gained in the course of systematic reactivity analysis of important reagents.

(4) Application: While technological application seems to be the dominant aim of preparative research from the layman's perspective, chemists are actually very restrained in explicitly referring to this aim. Since patents are the usual form for publishing applied research, application relevance in chemical journal papers is to be defined in a broader sense. Besides the authors' explicit expectation that the new substance might be useful in various technologies (energy, food, agricultural, medicine, chemical engineering etc.), it is also registered, if authors are looking for extraordinary physical (e.g. optical, electrical, magnetical) or biological properties.
(5) Structure typology: A peculiarity of chemists' interest in new substances is their preference for extraordinary structural features, that are recognizable after theoretically interpreting various measurements of the substance. Emphasis is laid on the structure of the nuclei (strange bond length and angle, symmetry, coordination sphere, structure dynamic etc.) as well as on the structure of electrons (non-classical bonding, unusual charge distribution, conjugation, mobility etc.). These features are extraordinary with regard to some structure typologies of ordinary or well-known substances but not with regard to the fundamental substance classification. And since they do not challenge up-to-date theorie these cases cannot be assigned to theory relevance too. They rather seem to prepare a classificatory approach on the theoretical level of structure.

Content analysis of the 300 papers was carried out by searching the whole text for given reasons corresponding to the relevance groups. At most three reasons per paper were registered, which was sufficient since more than 90% of the papers contain less than 3 reasons. In exceptional cases two reasons of one relevance group were registered, if they were strictly independent of each other. The mean number of reasons per paper is relatively stable at about 1.35 during the period of investigation and without significant difference between organic and inorganic papers.

3.2. Determining the methods of preparative chemistry

Whatever the production of new substances may be of use, the first problem of preparative chemists is how to produce them. To get more insight in preparative methods on a general level, a second content analysis was made. All 300 papers were searched for statements about instructions that lead the authors to successful preparations. The papers were classified into 5 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 in analogy to a former preparation of one of the authors according to a reference ("self-analogy");
(4) preparation is carried out in analogy to a former preparation of another author according to a reference ("other analogy");
(5) preparation was planned (not reconstructed) on the theoretical level of reaction mechanisms.[14]

Since details about instructions are expected to be of central significance in preparative chemistry, there is some evidence that a lack of statements (1) frequently corresponds to lack of referable instructions (2). This point is also supported by a linguistic analysis of peer reviews of the *Angewandte Chemie* pointing out that referees tend to discredit terms like "surprisingly", "contrary to expectations" etc.[15] In cases of lack of referable instructions we may suppose that preparation is carried out either by some intuitive access or by a combinatoric trial and error approach (cf. Part I, Sect. 4.2.4). Analogy preparation, on the other hand, depends on the transfer of experimental rules. The distinction between self-analogy (3) and other analogy (4) is made to distinguish between different status of rules on the average. While self-analogy may be possible on the basis of implicit laboratory rules or skills trained within a research group, other analogies depend on explicit rules transferred by (written) communications of scientific standard. Finally, instructions by reaction mechanisms (5) are based on explicit and general rules on the theoretical level of chemical structure theory.

4. Results

4.1. Aims of preparative chemistry

The results of the aim analysis are presented in Fig. 1. The main activity (42–45%) of preparative chemistry occurs in order to improve preparative abilities (synthesis relevance) by finding new reagents and catalysts, new experimental and theoretical methods. The relevances of theory, classification, and structure typology are much less important, while the former two are also decreasing. In the second place is application relevance which is rapidly growing. A detailed analysis reveals that the trend is for the most part due to the internationalization of the journal (Sect. 2.2). In North American communications of the years 1990 and 1995 application relevance is at 36% which is significantly higher than in German (24%) and other European (26%) communications of the same period.

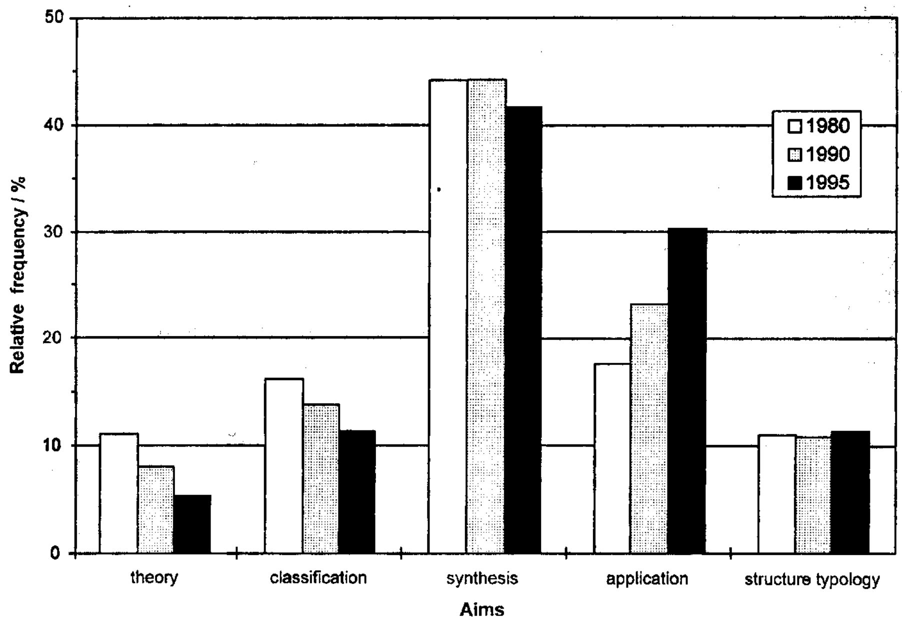

Fig. 1. Relative frequencies of aims in preparative chemistry each for the years 1980, 1990, and 1995

A comparison of communications from institutes of organic and inorganic chemistry (Fig. 2) shows that organic chemists have even a more clear-cut preference for synthesis relevance and application relevance (especially biological properties, medical and agricultural applications), other aims being almost negligible. The aims of inorganic chemists, on the other hand, are more heterogeneous. Besides synthesis relevance, special interest is also in opening up new substance classes (classification) and extraordinary structural features.

A closer look upon synthesis relevance indicates that half of the organic chemists engaged in that field are concerned in developing new experimental methods, some 20% are each looking for new reagents and reaction mechanisms, respectively, and 10% are carrying out systematical reaction tests. In contrast, the majority of inorganic chemists engaged in synthesis relevance are searching for catalysts for organic (!) synthesis, another quarter are establishing experimental methods frequently based on the use of catalysts for organic synthesis too; and while developing reaction mechanisms is almost negligible, systematical reaction tests are carried out at some 20%.

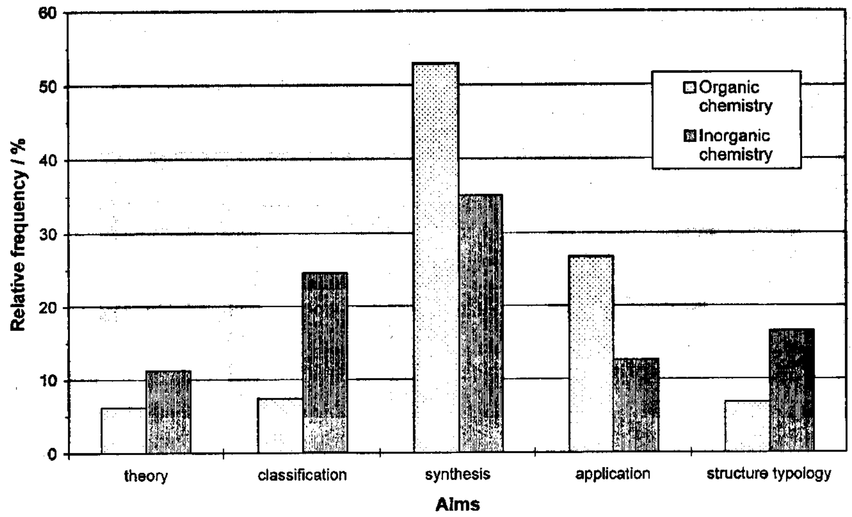

Fig. 2. Relative frequencies of aims in preparative organic and inorganic chemistry (all years considered)

4.2. Methods of preparative chemistry

There is a contrary tendency in organic and inorganic chemistry concerning the methods or instructions to prepare new substances (Fig. 3). Organic chemists prefer established instructions on the level of theoretical models (reaction mechanism, 36%) and explicit experimental rules (other analogies, 26%). The great majority of inorganic papers, on the other hand, do not refer to established instructions at all (no statements and no instruction, 53%) or refer to former preparations of their own (self-analogy, 28%).

If a lack of statements corresponds to a lack of referable instructions, as supposed in Sect. 3.2, then more than half of the successful preparative research of inorganic chemists would be done by an intuitive or combinatoric trial and error approach; in organic chemistry this would be at least 22%. If we group self-analogy and other analogy together, then analogy preparation is carried out at 43% in inorganic and at 41% in organic chemistry. While theoretical instructions are of central importance in organic chemistry (36%), they are actually negligible in inorganic chemistry (3%).

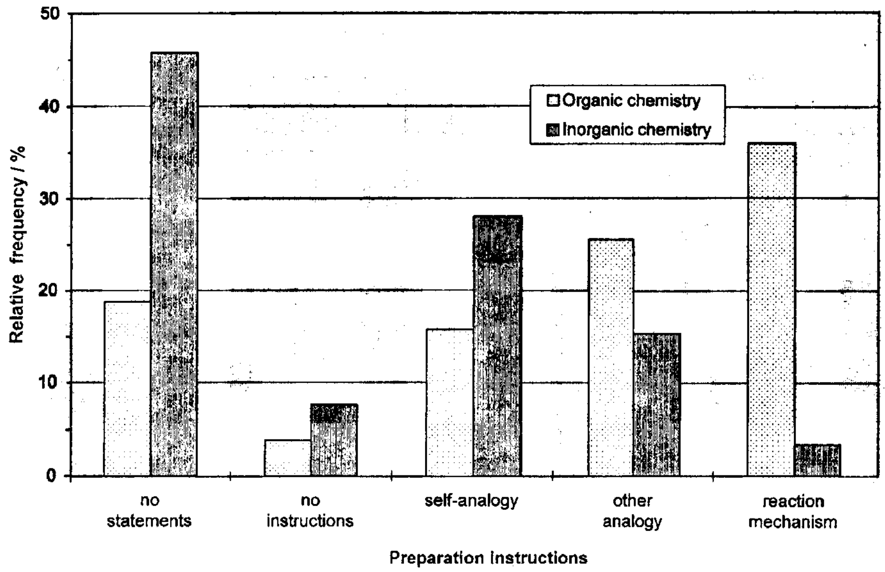

Fig. 3. Relative frequencies of instructions in preparative organic and inorganic chemistry (all years considered)

4.3. Frequency distribution of the number of new substances

In organic chemistry the mean number of new substances per paper is twice as large as in inorganic chemistry (Table 1). Moreover, the frequency distributions of the number of new substances (n) are quite different in these fields (Fig. 4). A third of inorganic papers report only about one new substance. The frequency distribution rapidly decreases with higher substance numbers corresponding to a 1/n-distribution (until n=3 the decline even corresponds to a Poisson distribution). On the other hand, the frequency distribution of organic chemistry papers is very flat and shows several maxima without any significant correspondence to statistical distributions. While 15% of organic papers each report about more than 10 new substances, less than 1% of inorganic papers do so.

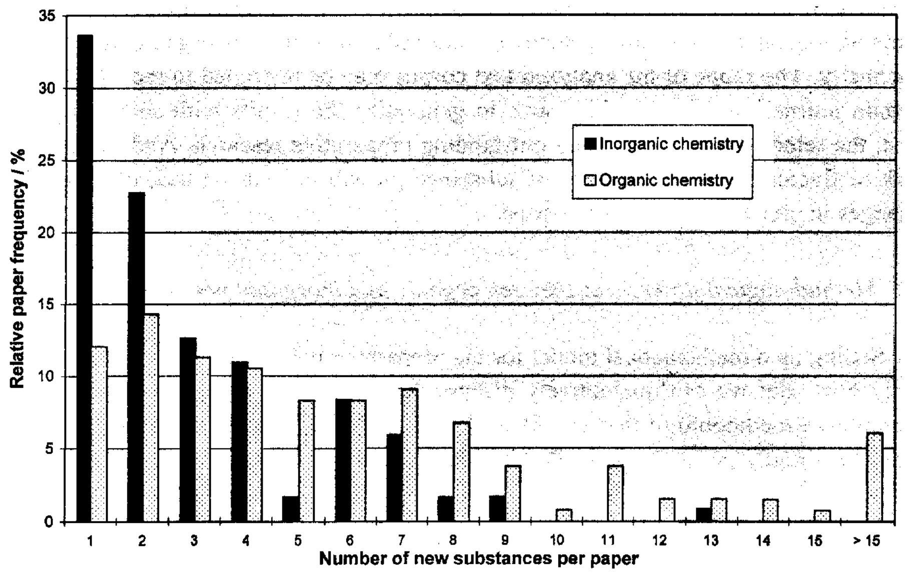

Fig. 4. Relative frequency distributions of the number of new substances in communications of preparative organic and inorganic chemistry (all years considered)

Inorganic chemists obviously prefer "one-substance-papers". A single new substance is frequently sufficient for their main research aims (e.g., a prototype of a new substance class, structural features, a new catalyst). Further new substances are often side-products that are easily accessible by analogy preparation. On the other hand, the main research aims of organic chemistry frequently require the production of a couple of new substances: The capacity of a new synthetical method is extensively proved, a new substance with biological activity is diversely modified to find the most active derivative etc. Moreover, theoretical synthesis strategy for a certain target molecule often includes a series of new substances as intermediate steps.

5. Discussion

As has been pointed out in Part I, there is a rapid exponential growth of chemical substances during the past 130 years that is mainly due to the growth of organic substances with annual growth rates at 5.5%, while inorganic substances, on the other hand, are growing at less stable and lower rates (on the average, 2.9%). The results of the content analysis enables us to understand the preparative research process in general methodological terms of aims, methods, and efficiency both of organic and inorganic chemistry. The scope of the analyzed text corpus may be restricted to recent papers of a certain journal, but we are able, now, to generalize the results with some care, since, first, the selected papers represent outstanding preparative research. And, secondly, the lack of fluctuations of the curves of substance growth indicates a lack of fundamental changes in preparative research process.

5.1. Methodological differences between organic and inorganic preparative chemistry

Setting up a mathematical model for the preparative research process is certainly too early now. But we can qualitatively discuss the results in correspondence to an ideal preparative methodology that would lead to exponential growth of maximum growth rate. As already pointed out in Part I (Sect. 4.2.4), exponential growth requires that preparative abilities grow hand in hand with the number of substances. Our *methodological model* is expected to correlate both developments in terms of aims and methods. The most efficient increase of chemical substances would be achieved, if:

(1) The production of new substances occurs in order to improve preparative abilities on the level of (a) tools (reagents, catalysts, etc.), (b) experimental methods, or (c) theoretical methods.

(2) The production of new substances is actually guided by results of former research 1 a–c.

(3) Research according to the aims 1 a–c requires the production of many new substances.

It should be emphasized that, according to this methodological model, the relationship between researches of different times is not superficial in that the later is by chance "inspired" by the former. Instead, the former research is *intended* to enable the later which in turn necessarily *depends* on the former. Thus the methodological model describes an ideal diachronic co-operation in the sense of an extended and coherent research program.

As the most important result, preparative research in organic chemistry approximately complies with all three conditions. New substances are principally produced with the explicit aim to improve the abilities for further production of new substances with special importance of level b (Sect. 4.1); (the role of application relevance will be discussed in the next section). Organic chemists extensively use former results of experimental and theoretical methods as instructions for their own preparative research (Sect. 4.2). And their specific aims actually require the production of many substances (Sect. 4.3). Since organic preparative chemistry approximates our methodological model of an ideal preparative science, we are not surprised at the rapid exponential growth of organic substances.

Preparative research of inorganic chemists, on the other hand, seems to be methodologically heterogeneous. They are less interested in the improvement of their own preparative abilities but rather in the discovery of catalysts for organic synthesis. They have quite different specific aims (classification, structural features) that do not require the production of many new substances. Moreover, specific methods to open up a new substance class or to find certain structural features are still hard to find, so that there are only little references to established methods. Consequently, the growth of inorganic substances is much slower and less stable. Nonetheless, there is also exponential growth on the average, which can be explained on the level of material resources. Since every substance can serve as a starting point for chemical synthesis at least by the combinatoric approach (cf. Part I, Sect. 4.2.4), preparative capacity grows along with the number of known substances.

5.2. Preparative chemistry between pure and applied science

According to the ideal methodological model, multiplying chemical substances is considered as an end in itself. In this regard, preparative organic chemistry seems to be approximately a pure science, comparable to the classical pursuit of truth. But thusfar we have neglected application relevance that seems to be of considerable and increasing significance too. Should we take technological application as the underlying or final aim of the whole enterprise of preparative chemistry? There is actually no empirical evidence that application relevance is the leading idea. Certainly, we cannot measure application relevance of preparative chemistry by considering chemical journal papers only, because the patent system provides an own publication form for this field. But as has been pointed out in Part I (Sect. 4.2.3), there is no correlation between patent rates and preparative productivity. Moreover, while application relevance seems to be increasing, the number of patents per new substances is actually not but rather decreasing since about 1985. Hence, the increase of uttered application relevance is assumed to be an effect of rhetorical change.

However, application relevance is undoubtedly important at least in preparative organic chemistry. So we may finally raise the question whether there is a conflict or some other (internal) relationship between the two aims, i.e., between pure and applied preparative research. From the application point of view the numerical increase of substances is a senseless enterprise, unless research is restricted to substances of possible use. From the point of view of pure science, on the other hand, such a restriction would be intolerable. Hence we would expect a conflict between the two aims at first glance. In preparative chemistry, however, a parallel orientation towards pure and applied research is not only easy-going, it can even improve the former. Take the increase of chemical substances as the aim of pure preparative research, then research is more efficient, if many scientists (synchronically and diachronically) co-operate in the same field of substances and methods (Sect. 5.1). A common interest in applications of a certain substance field concentrates research activity, which would be more disordered otherwise. Hence, as long as application relevance is not too narrow, it even benefits pure preparative research.

6. Conclusions

Chemistry, as today's main active science, is for the most part concerned in producing and characterizing new substances. There is still no saturation discernible after 200 years of exponential growth of substances. Of that by far the major part are produced by organic chemists. The different productivity of organic and inorganic preparative chemistry can be explained by different methodological patterns set up from results of the content analysis of recent papers. While the latter have diverse aims and strategies, organic chemists approximates an ideal preparative methodology. Their main purpose of producing new substances is the improvement of preparative abilities on different levels for further substance production, i.e. multiplying chemical substances is an end in itself. The respective substance field may indeed be also affected to a certain extent by actual non-scientific needs, interests in application, and fashions, but the end in itself seems to be stable until today. Of course, one might question whether this self-referential research process is efficient for needs outside of science, but it is undoubtedly highly successful inside.

Notes

1. *Schummer*, 1997; this is referred to as "Part I" below.
2. The philosophical neglect of chemistry is discussed in detail in *Psarros* et al. 1996; the "invisibility" of chemistry from the general perspective of cultural studies is dealt with in *Mauskopf* 1993.
3. Standard bibliographies of bibliometrics (*Hierppe* 1980, *Prichard* 1981, *Sellen* 1993) list some 100 titles on chemistry which are not even complete. Since 1918 there are regular communications by the editors of *Chemical Abstracts*, mostly in *Chemical Engineering News*. From 1960 till 1974 there was even an own *Journal of Chemical Documentation*, later dominated by computational chemistry. Within

chemistry, analytical chemistry is the most prominent topic of scientometric studies, mostly published in chemical journals; cf., e.g., *Braun* et al. 1980 and quoted literature.

4. Cf. *Grissom* 1991; *Daniel* 1993b, p. 9f. The ISI chemical journal impact factors have been questioned and corrected by *Braun & Glänzel* 1995 and *Moed* et al. 1996.
5. Cf. *Daniel* 1993b, pp. 35–42 and *Daniel* 1993a, p. 248f. regarding the year 1984. His comparison between offered and published manuscripts shows that the thematic profile is already pre-shaped by the offers.
6. Chemical Abstract Service 1996; reference data are calculated by dividing the number of new substance by the number of new papers a year (cf. Part I, Fig. 4).
7. Cf. also the editors' statistics on offered and published manuscript (*Brunner* 1995).
8. Notice, that the distribution is still far from being quantitatively representative according to *Chemical Abstracts* for the year 1995 (Germany, 7.7%; other European countries (without Russia), 20.1%; North America, 30%; all others, 42.2%).
9. The data were supplied by the chief-editor P. Gölitz. Notice, that the peer review system was introduced in 1982.
10. *Daniel* (1993b, pp. 33–35) points out that peer reviewer have a little but significant preference for manuscripts submitted by authors of higher academic status.
11. Notice, that the rate of female authors in preparative chemistry did nearly double but is still very low.
12. Of exceptional state is, however, the field of technological aims, for this is covered by the publication system of patents. This will be discussed in Sect. 5.2.
13. If theoretical concepts are explicitly aimed at solving classifiatory or synthetical problems, this is considered in the corresponding group (s.b.).
14. Notice that, opposite to a widely held opinion, quantum mechanics hardly enables chemists to prepare new substances today. In fact, not a single of the 300 papers under investigation refers to any quantum mechanically based hint or instruction.
15. *Kretzenbacher & Thurmair* 1992, p. 140.

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