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SCIENTOMETRIC STUDIES ON CHEMISTRY I: THE EXPONENTIAL GROWTH OF CHEMICAL SUBSTANCES, 1800–1995

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The number of chemical substances is considered as a cumulative measure of the cognitive growth of preparative chemistry. During the past 200 years there is approximately exponential growth without saturation. Separate analysis of organic and inorganic chemistry suggests at least a two-phase model either. Detailed discussion of the results (considering also the growth of chemists, chemical papers, patents, and chemical elements) reveals that an external (socio-economical) explanation is insufficient. Instead, an internal (methodological) approach is suggested to explain the exponential growth as well as balancing phenomena in war and post-war times.

1. Introduction

Since Price's pioneering studies on the growth of science, a great deal of work has been done on bibliometrics, both refining its methods and applying them to various scientific fields. Certainly, the success is due to its wide applicability abstracting from any specific cognitive content of the science under investigation. On the other hand, serious objections have been raised, whether bibliometric indicators, e.g., the number of journal articles, do reflect the *cognitive* development of science at all.[1] Since *Kuhn*'s (1962) and *Feyerabend*'s (1970) studies on the philosophy of science any cumulative picture of scientific knowledge even appears to be 'philosophically incorrect'. Moreover, abstinence from any cognitive content confines scientometric studies on growth to a phenomenological level, unless the growth of scientific activity is simply explained by the growth of scientific activists.[2] For explanations of pure activity data in *cognitive terms* of "births of advances", "stimulus for discovery", "epidemic transmission of ideas" etc.[3] either presuppose a cognitive explanandum that has not yet been measured, or are non-explanatory metaphors.

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Supplementary to bibliometric studies on scientific activity, special investigations of the *growth of scientific knowledge* are in need. Unfortunately 'cognitive units' allowing a cumulative measure of scientific knowledge are difficult to ascertain in many disciplines. However, access is possible with regard to classificatory sciences based on stable classificatory systems. Since many centuries systematic zoologists, botanists, chemists etc. are collecting much of their knowledge cumulatively corresponding to a (literal) accumulation of their species. These sciences are far from being marginal but rather the most active sciences with regard to bibliometric indicators;[4] and, as will be pointed out later, the discovery/production and characterization of new species is actually a major task at least in chemistry. While the growth of zoological species has already been analyzed (*Simon* 1982), a respective study on chemistry is still missing.

In this paper I shall first present data of the growth of chemical substances during the past two hundred years collected from many well-known handbooks. A detailed discussion of the results (including additional data sets about the number of chemists, chemical papers and patents) will reveal that external (socio-economical) explanations of the growth are insufficient. Instead, I shall propose three internal or methodological models that make the exponential growth of chemical substances more plausible and may contribute to an innovation theory for preparative chemistry. In a subsequent paper the research process of producing new chemical substances will be investigated in more detail by content analysis of chemical journal papers (*Schummer* 1997).

2. Collection of data and error estimates

Since a couple of centuries chemists are used to systematize their knowledge in handbooks according to chemical substances. Authors of chemical handbooks have always attached importance to the point that the actual material diversity is reflected either in the table of content or in an appended index of substance names. Hence, counting up tables and indexes of appropriate handbooks of the past 200 years should yield a rough quantitative picture of the growth of chemical substances, and, since the overwelming majority of substances are synthesized in the laboratories, it will also give insight in the research of preparative chemistry.

Exact data about new chemical substances are available since 1965, when the *Chemical Abstract Service* (CAS) has developed a sophisticated registry system assigning every new compound a registry number.[5] Prior to 1965 only Richter's three handbooks provide exact data of organic substances described in chemical literature until 1883, 1899, and 1910, respectively.[6]

To collect further data the entries of organic and inorganic substance names were separately counted from indexes of well-known chemical handbooks. Random sample surveys were carried out for handbooks after 1850 considering possible fluctuations of entry density (due to the systematical or alphabethical order); errors are estimated less than 5% (α=0.05). In addition one published estimate of the number of organic substances of the year 1937 is considered, because of the lack of available data in the midth of 20th century.

On the time axis the relevant year is fixed by the date of the last volume's completion or close of literature analysis if discernible, otherwise by the year of publication. In special cases (6th and 7th edn. of Gmelin's handbook) additional volumes published with considerable delay (as a consequence of a war) are neglected, if the error is estimated less than 5%. On the whole, the error due to the different and sometimes extended periods of editing is expected to be higher than the error due to the sample survey, because the mean annual growth rate of chemical substances is about 5.5%.

Certainly there are remarkable discrepancies between handbooks or authors of different ages both concerning their criteria and scopes for recording chemical substances. In adjustment to later criteria only systematical inorganic substance names (no trivial names, no minerals) and only names of pure organic compounds (no unspecific natural products like oils, resins, essences etc., no organo-metallic salts) are considered in handbooks of the first half of 19th century. Special problems arise in organic chemistry when isomers and derivatives are not recorded separately, which is the case, for instance, in the editions 1–4 of Beilstein's handbook.[7] Fortunately this period is also covered by the more complete handbooks of Richter.

Following Berzelius' influential distinction between organic and inorganic chemistry organo-metallic compounds were no longer indexed from the second edition of Gmelin's handbook till the 20th century, when organo-metallic chemistry was booming. On the other hand, because the two subdisciplines have been nearly independently developed during that period, there was also little preparative work in the intermediary field of organo-metallic compounds, so that the neglect of indexing them is supposed to be of little consequence. In general, sophistication of the indexes (e.g., separate entries of different isomers) goes roughly along with preparative activity in the respective area. Therefore, the resulting error is expected to be at most a little temporal displacement of the curve.

First or unique editions of handbooks are probably based on a more restricted scope of chemical literature than succeeding editions, so that the number of recorded substances is rather too small. This is obviously the case with the first editions of

Beilstein's handbook, that are not considered in the present context, compared with the contemporaneous and more complete ones of Richter. The same probably goes for the first edition of Richter's and the unique edition of Weltzien's handbook.

Figure 1 shows the resultant data of the number of organic and inorganic substances in semi-logarithmic scale. Addition of the linear interpolation of both data series yields the development of all chemical substances until 1959 (last completed edition of Beilstein's handbook). Because the CAS registry system only registers the *new* substances of each year from 1965 on, the CAS data must be adjusted to the curve by calculating a basic value for 1964.[8] That provides, for the first time, a quantitative picture of the growth of chemical (inorganic and organic) substances during the past 200 years.

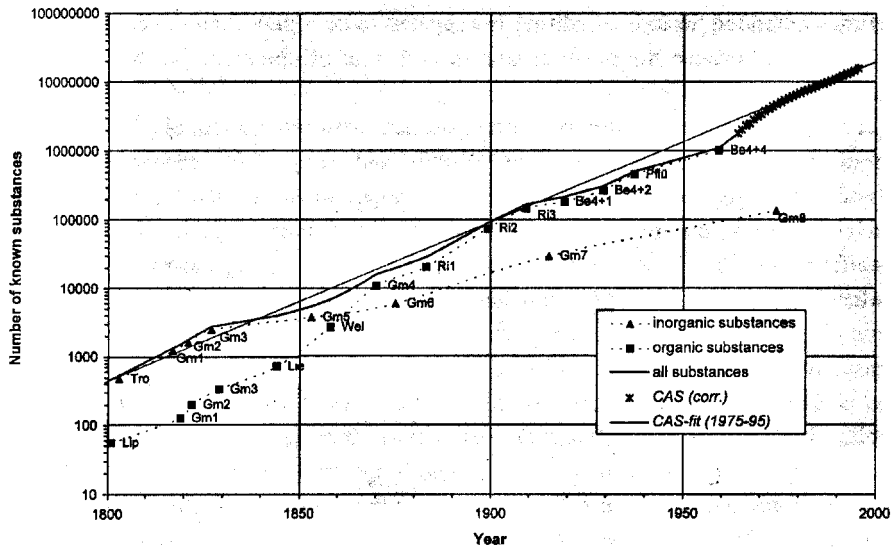

Fig. 1. The growth of chemical substances during the past 200 years from various sources: **Lip**: E.O. von Lippmann, *Zeittafeln zur Geschichte der organischen Chemie*, Springer, Berlin, 1921; **Tro**: D.J.B. Trommsdorff: *Systematisches Handbuch der gesammten Chemie*, Hennings, Erfurt 1800–7; **Gm1–8**: Gmelins *Handbuch der theoretischen/anorganischen Chemie*, edns. 1–8, 1817–1980; **Lie**: J. Liebig, *Traité de chimie organique*, Fortin, Paris, 1840–4; **Wel**: C. Weltzien, *Systematische Zusammenstellung der organischen Verbindungen*, Vieweg, Braunschweig 1860; **Ri1–3**: M.M. Richter, *Lexikon der Kohlenstoffverbindungen*, edns. 1–3., 1884–1912; **Be4+1/+2/+4**: *Beilsteins Handbuch der Organischen Chemie*, 4th edn., *General-Formelregister für das Hauptwerk und das 1./1.–2./1.-4. Ergänzungswerk*, Springer, Berlin 1939–1992; **Pflü**: M. Pflücke, *Angewandte Chemie*, 50 (1937), 957; **CAS (corr.)**: *CAS Statistical Summary 1907–1995*, Columbus/Ohio 1996 (adjusted data); **CAS-fit**: line fitted to adjusted CAS data of the years 1975–95

3. Results

The curves in Fig. 1 show at least five remarkable features of the chemical substance growth:
(1) During the whole period the *total curve* corresponds quite well to a stable exponential growth (i.e. a straight line in semi-logarithmic scale) with an annual rate of 5.5% and doubling time of 12.9 years.
(2) During the past 20 years (1975–95) the *total curve* corresponds *nearly exactly* to this exponential growth without any sign of saturation. Notice, that in figure 1 the straight line is calculated by linear regression of the logarithmic CAS data of years 1975–95 (r=0.9995) and will be referred to as the "ideal exponential growth" below.
(3) Since about 1840 the total curve shows only four obvious *deviations* from the ideal exponential growth all being temporarily negative: (a) 1840–70, (b) 1870–90, (c) 1915–37, (d) 1937–70.
(4) During the first seventy years of the 19th century the number *of organic substances* rapidly increases from a very low level in two steps (1800–25, 1825–70). Since about the 1870s the total curve is decisively determined by the growth of organic substances.
(5) After a period of rapid growth in the first three decades of the 19th century the number of *inorganic substances* nearly stagnates for some thirty years loosing its dominant influence on the total curve. Since then the growth of inorganic substances is relatively stable with mean growth rate of 2.9% (doubling time: 24.3 years).

4. Discussion

The results suggest that the discussion is reasonably divided up in two periods: The curves of inorganic and organic substances show obvious fluctuations until about 1870, whereas the development is relatively stable afterwards.

4.1. Dynamics of preparative chemistry 1800–1870

During the first third of the 19th century preparative *inorganic chemistry* is basically influenced by two new classificatory approaches. First, the "new" (anti-phlogiston) chemistry of Lavoisier et al. proposed a new system of nomenclature and classification that rapidly spread over whole Europe.[9] Initially based only on few well-known substances in a rather speculative manner,[10] the classificatory system predicted

a great deal of new substances which could easily be produced in the laboratory by analogical combination procedures. Trommsdorff's handbook and Gmelin's first three editions mainly reflect the procedure of filling classificatory gaps by schematically combining various acids with various metal oxides (e.g., "arsenigsaures Eisenoxidul"). Secondly, the law of multiple proportions suggested a quantitative approach combining different elements in various mass proportions (e.g. "Doppeltschwefel-Antimon", "Drittehalbschwefel-Antimon" etc.) Both combinatoric approaches were further accelerated by the discovery of many new chemical elements (Fig. 2) multiplying the number of possible combinations. In the late 1830s the combinatorical approaches were likely to be nearly exhausted. Moreover, the discovery of new elements was rare in the following decades (Fig. 2), so that the curve gets flatter. Further growth of inorganic substances depended on the invention of more sophisticated but less universal preparative methods and the discovery of new (and stable) elements.

The curve *of organic substances* reveals two distinct periods of over-exponential growth. During the first period (1800–25) there was an increasing interest in the analysis of animals and specially plants by means of destillation and extraction. At that time expeditions to remoted parts of the world collected rich material for chemical analysis. Chemists were highly interested in exploiting natural products like oils, resins, dyes, essences, waxes, rubbers etc., so that the number of corresponding entries rapidly increased. Beside these unspecific natural products (which are not considered in the present context), chemical analysis also yielded pure substances as by-products (crystallized solids, liquids with definite boiling point). In the late 1820s (when some 200 pure organic substances were known) chemists took a more systematic interest in these substances trying to characterize them by sophisticated techniques of elemental analysis. The transition from the first (analytical) period to the second (synthetical) period required two important steps. First, the overcoming of the metaphysical dogma that organic substances are part of the organic realm reigned by *vis vitalis* and inaccessible by pure laboratory synthesis. And secondly, the development of a classificatory approach that includes hitherto unknown substances and points at experimental ways of synthesizing them. While vitalism was shaked by Wöhler's synthesis of urea, chemists developed two competing classification approaches (radical and type theory) that guided chemical synthesis from then on. Similiar to the first decades of nineteenth-century inorganic chemistry, the second period of organic preparative chemistry seems to have been mainly the task of filling obvious gaps of the classification system by combinatorical and analogical procedures (e.g. combining various types with various residues). There were doubling times of some seven years in the 1850s and 1860s, before the approaches seem to have been suddenly exhausted.

Ironically, the exhaustion of preparative activity coincides with the development of structure theory in the late 1860s, which is actually the theoretical basis for any further preparative research in organic chemistry.

Until about 1870 the total curve can be explained by different research trends in organic and inorganic chemistry. In both cases we find classificatory approaches fruitfully guiding preparative activity by combinatoric and analogical reasoning until saturation.[11] Subsequent periods show lower but more stable exponential growth in the long run. The transition from inorganic to organic chemistry as the dominant preparative subdiscipline explains the first temporary negative deviation of the total curve (1840–70).

4.2. Dynamics of preparative chemistry 1870–1995

4.2.1. Exponential growth and catching-up phenomena.

From about 1870 to the present all curves reveal a relative stable exponential growth of chemical substances. Each significant deviation of the total curve from ideal exponential growth is temporarily negative and obviously related to wars (French-German war, World War I and II) with regard to the beginning, extent and duration of the deviation.[12] In war and post-war periods socio-economical conditions of research are ordinarily reduced (research funds are cut down, scientists are ordered off, publication and education systems break down, results are kept under lock, potential scientists of the next generation are sacrificed etc.). Thus *without effects of war we would expect an ideal exponential growth of chemical substances.*

But, surprisingly, in times of war we do not find temporal displacements of the growth as we are used to find in many social and even scientific developments (see, e.g., Fig. 3). Instead there are only temporary deviations from the *same* exponential curve of the whole period. Chemists seem to catch up the war effected loss till the ideal curve is approximated, which is most obvious in the past fifty years. Three possible explanation for this *catching-up phenomenon* may be hypothesized: (1) In post-war times chemists make additional efforts in preparative research until they reach either (a) an consciously set goal, or (b) an externally determined limit of growth. (2) In times of war basic preparative research (development of new methods) still continues, whereas routine application and publication is put off for post-war times of rich resources. Because of a lack of quantitative goals (as a lack of known data) we may unquestionably drop explanation 1 a. Hence, the exponential growth is determined either by external (socio-economical) factors (1 b) or by internal (methodological) factors (2).

In what follows I will exclude pure external approaches before proposing methodological explanations for the exponential growth of chemical substances. But first we should question the view, that exponential growth of science is self-evident.

4.2.2. Is exponential growth self-evident? The case of chemical elements.

Price found exponential growth in science as a "fundamental law",[13] which he (roughly) verified by the growth of scientists, universities, journals, abstract journals, papers and so on. But unlike these social and organizational parameters, chemical substances are substantial results of scientific research that need not to obey the laws of social growth. An instructive counter-example from chemistry is the history of the discovery of chemical elements showing roughly a *linear growth* during the past 200 years (Fig. 2).[14] The history of discovery may easily divided up in a series of different research programs each initiated by some methodical innovation that was exhausted very soon in most cases.[15]

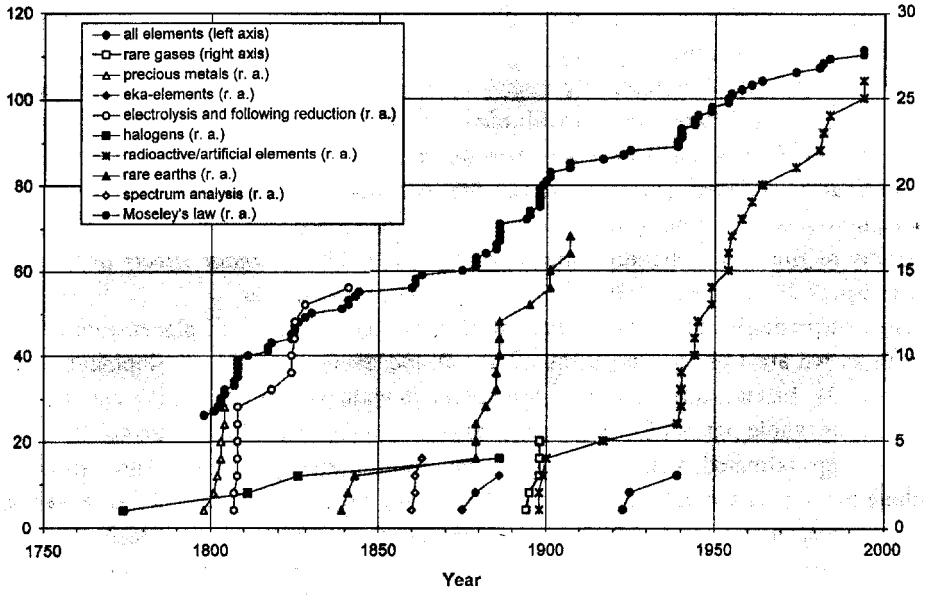

Fig. 2. Discovery of chemical elements (data from various source of the history of chemistry)

After establishing the new operational definition of chemical elements in 1789 (25 elements in the modern sense were known hitherto), the most important precious metals were gained by glowing the oxides within 7 years. The history of discovery of new elements by spectra analysis (Cs, Rb, Tl, In) was finished in 4 years. The rare gases were discovered in 6 years. Predictions of Mendeleev's "eka-elements" (Ga, Ge, Sc) and Moseley's law (Hf, Re, Fr) were confirmed by chemical discovery in 12 and 17 years respectively.[16] Of exceptional length is the story of the (early predicted) halogens lasting more than hundred years. Over and above that there are three following innovations: After establishing the electrolytic method to gain alkali metals and earths some of the resultant new elements were used to reduce metal oxide for discovering further elements (e.g., Zr, Si, Al, Ti, Be). Some forty years after discovering the first rare earths some of these putative elements appeared to be separable, whereupon a following analytic program yielded 13 more elements. Discovery of the first radioactive elements reveals the composed character of elements as a basis for the physicist's program of artificially making new elements some 40 years later.

According to Rescher's patterns of scientific growth, linear growth (like the growth of elements) is restricted to "first rate" topics, whereas exponential growth with annual rates of more than 5% (like the growth of chemical substances) is, on the other hand, "routine" research.[17] The history of chemical elements gives us more insight in such "first rate" research: The linear growth of elements is due to a linear rate of exhausting innovations (about one innovation per 15 years), in which following innovations are exceptional.

How can we shift from linear to exponential growth of products? Two ways can be hypothesized. (1) If innovations are exhausting, then we need an exponential growth of innovations;[18] this would be the case, if each innovation sets off more than one following innovation on average. I will call this the "creative" or "internal" way. (2) If innovations are not exhausting, then we need a single innovation only that may be exploited by exponentially increasing capacity of "routine" work. In this case, exponential growth is simply caused by an exponential growth of man-power. This will be referred to as the "routine" or "external" way. Certainly the difference is not such as strict as it seems to be at first glance. The difference between exploiting a single innovation and developing a new one by some transfer is rather a gradual one depending on the scope of analogy transfer. But we may settle the difference in operational terms: If we do not find any significant correlation between the growth of products and external factors (socio-economical conditions like man-power), then the external or routine way is extremely unlikely.

4.2.3. Questioning the externalist explanation of exponential growth.

At first glance, data reflecting the development of chemical research activity seem to support the external explanation of the growth of chemical substances. We actually find extended periods of exponential growth of chemists and chemical publications during the 20th century interrupted in war times only (Fig. 3).[19] However the meaningful terms are the quotients (new substances per chemist and year, new substance per article) in Fig. 4. Here we find considerable fluctuations. In post-war times (1950–64), when deviation of the total substance curve is at most (Fig. 1), the mean substance productivity of a chemist rises at four times the high (Fig. 4). A similiar but much weaker movement was already in the period between the wars. And productivity decreases in the late 1960s just at time, when the substance curve reaches the ideal curve. In the late 1970s the growth rate of chemists decreases to 3.3% (Fig. 3). The decrease was again compensated by higher productivity in the 1980s, so that the 5.5% growth rate of chemical substances could be stabilized. All these phenomena are in conflict with the external explanation. Moreover, they seem to indicate a kind of balancing process with compensation phenomena in *both* directions that makes the idea of an external resource controlled process unreasonable.

Multiplying the chemical substances is a central aim of chemists. This is clarified when the number of new substances per article and chemists' article productivity are considered (Fig. 4). The number of new substances per chemically relevant article has been doubled in post-war times and ranges between 1 and 1.7 (!) later, although the article productivity per chemist has similarily increased in the same period. And while chemists' mean article productivity is decreasing since the late 1970, that does not affect at all their mean substance productivity, so that the number of new substances per article is strongly increasing. What ever the reason of the decline of article productivity may be (limits of the publication system, higher publication standards, less research motivation etc.) it does not prevent chemists from further multiplying their substances corresponding to the ideal curve.

From the externalist point of view one might object that chemists's substance productivity is motivated by possible techno-economical exploitation. But this is obviously wrong, if we take the number of chemical patents as a measure of applied research. In fact, the number of patents per new substances (Fig. 5) went rapidly down in post-war times, and after a period of stagnation it is again decreasing in the last decade. The curves of patents per article and per chemist (Fig. 5) are quiet similiar, so that these trends may actually reflect chemists's mean interest in applied research. Since we find high substance productivity in times of low interest in exploitation and the other way round, chemists' preparative research cannot be controlled by their interest in techno-economical exploitation.

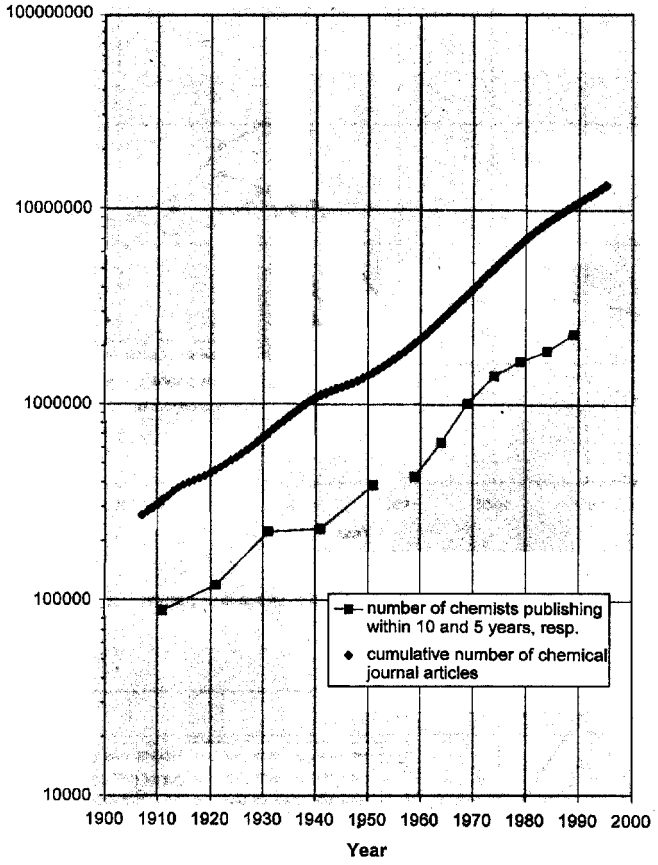

Fig. 3. Growth of chemists and chemical journal papers (basic data from CAS, the number of papers prior to 1907 is from *Tague* et al. 1981, p. 132 estimated according to *May*'s (1966) method)

The results make clear that a sociological explanation of the growth of chemical substances is difficult to find. Socio-economical conditions may actually be a limiting factor, if they fall below a critical value as it is in case of war times. But even then the effect is only a temporary one and seems not to affect basic preparative research, which is illuminated by the catching-up phenomena. Furthermore, analysis of the catching-up phenomenon reveals a kind of internal balancing process when approximating the ideal curve. Since chemists cut down their mean substance productivity just at time when the ideal curve is reached etc., the idea of an externally determined upper limit of growth (alternative 1b of Sect. 4.2.1) gets highly implausible.

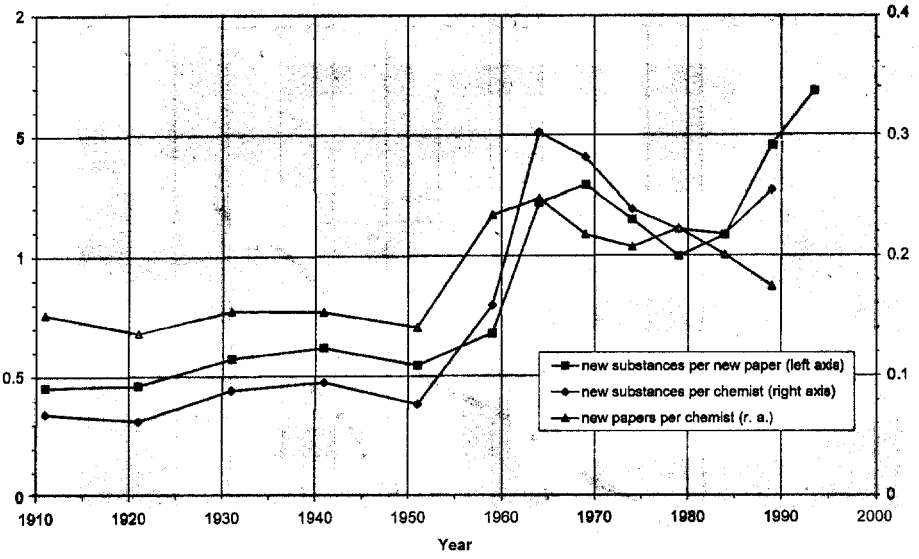

Fig. 4. Relative development of new chemical substances and papers (basic data from CAS)

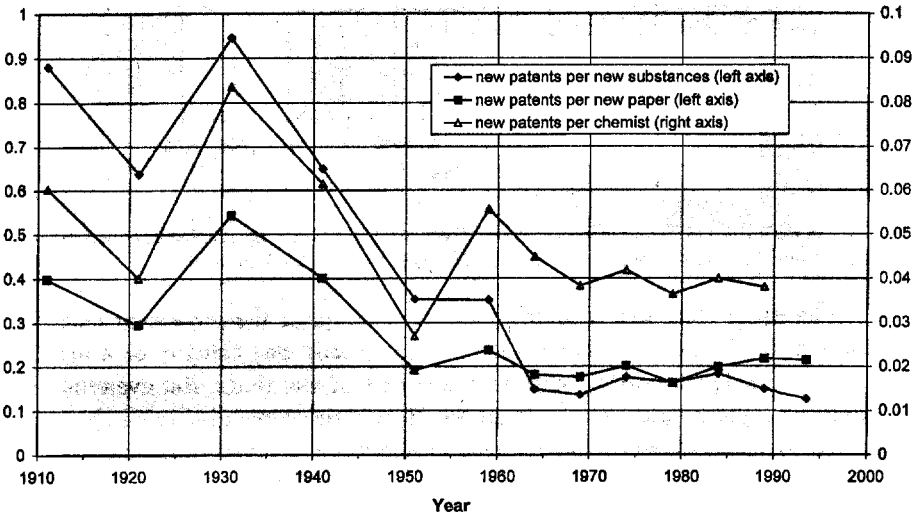

Fig. 5. Relative development of new chemical patents (basic data from CAS)

4.2.4. Methodological models for exponential growth.

The implausibility of external or sociological explanations supports the idea that the exponential growth of chemical substances could be guided by internal or methodological conditions of preparative research itself. But what kind of method might induce an exponential growth? To restrict free speculations we may fix general conditions in mathematical terms: Exponential growth means that the substance production rate (dS/dt) is a linear function of the number of known substances (S(t)) at any time, $dS/dt=k\,S(t)$. That would be the case, if either the known substances as tools or the knowledge how to prepare them basically enable chemists to produce further substances. Hence, we have already two methodological approaches:

(1) The method can be a simple *combinatoric approach.* New substances are produced by experimentally combining older ones. If n substances are known, then a new (n+1)th substance enables n new pair combinations. Exponential growth does not require, that every combination is successfull, we rather need a constant rate of success. But combinations should be restricted to pairs, because higher combinations would yield over-exponential growth.

The combinatoric approach has some plausibility, for chemical synthesis actually dependends on mixing known substances (frequently pairs). But oddly enough the success rate k should be constant during the whole period of exponential growth unaffected by instrumental and theoretical innovations. Moreover, since the combinatoric method appears to be the extreme of routine work, we would expect the growth of chemical substances directly reflecting the input of chemical man-power. But that is in conflict with our results. Combinatoric method was actually at work in early nineteenth-century chemistry (Sect. 4.1), and it is probably so until today in some areas of chemistry. But it cannot be the main method responsible for exponential growth in organic chemistry of the past 130 years.

(2) Since knowing a substance in chemical terms also means to know how to produce it, there is a set of recipes corresponding to the set of known substances at any time. Hence, we would expect exponential growth of substances, if the set of known recipes enables new preparations by analogy at a constant rate. The *analogy approach* equals the case of exponential growth of exhausting innovations in Sect. 4.2.2. Now, we can clarify the difference between routine work (strong analogy transfer) and innovation (weak analogy transfer) with regard to chemistry: Further substances of the same substance class are prepared by strong analogy transfer, i.e. slight modification of experimental conditions until the class is exhausted. Innovation occurs if a more radical modification of experimental conditions succeeds in opening up a new substance class. Exponential growth of chemical substances according to the innovative path would

require, that each innovation stimulates more than one exhausting innovation on average at constant rate. That is to say, that the set of former innovation remains an inexhaustible source for inspiring further innovations.

The analogy approach is able to explain catching-up phenomena, for preparative research is divided up in basic (innovative) research and routine (innovation exhausting) work. In times of low resources chemists may concentrate on basic research that can be exploited later at a higher level of resources until exhaustion (approximation to the ideal curve). Although the assumption of a constant innovation rate still needs further explanation, the model seems to be much more reasonable than the external approaches.

(3) There is still a third approach conceivable that explains the exponential growth of substance with regard to methodical innovations on the theoretical level of preparative chemistry. In general terms, if each new innovation has a positive feedback on every former innovation extending its scope, then a linear sequence of innovations is sufficient to yield exponential growth. The *feed back approach* presupposes a network of methods in which the capacities of preparative methods depend on each other. In fact, reaction types and mechanisms based on chemical structure theory of the late 1860s comply with this condition.[20] Until today the path between chemical substance classes is directed by reaction mechanisms in a more and more sophisticated way. Assume that A, B, C, D, E, F are substance classes, and R1 and R2 are reaction mechanisms leading from A and B to C (R1: A+B->C) and from C and D to E (R2: C+D->E), respectively. Then a new reaction mechanism R3 (D+F->A) would not only enlarge the number of class A substances. It would also increase the capacity of mechanism R1 multiplying the number of class C substances, which in turn would increase the capacity of reaction mechanism R3, and so on. As long as reaction mechanisms are sufficiently connected with each other, the innovative power of a new mechanism is expected to be roughly proportional to the number of known mechanisms. In this case, linear growth of reaction mechanism (cf. Rescher's "first rate" research) yields exponential growth of chemical substances.

Since the feed back model links exponential growth of routine research to linear growth of basic research, it is even more capable to explain catching-up phenomena. Moreover, there is also strong support from the history of chemistry. For the period of stable exponential growth of organic substances began just at the time when structure theory was established as the constant basis for reaction types and mechanisms until today. But we should admit that the assumption of linear growth of reaction mechanisms still needs further investigation.

5. Conclusions

Unlike 'formal' bibliometric indicators, the number of chemical substances can be considered as a cumulative measure of the growth of knowledge in preparative chemistry. Data collected from many handbooks of chemistry show, that there is an almost stable exponential growth during the past 200 years. A more detailed analysis reveals two distinct phases in the development of inorganic and organic substances either. The first phase is characterized by rapid and less stable growth in both cases. This can be explained by exploiting systematical accounts of combinatorical and analogical reasoning. (In early nineteenth-century organic chemistry there is also a preceding pre-synthetical phase, in which the discovery of new (pure) substances seems to have been a side-effect at first.) The second phase, which begins in the 1840s for inorganic and in the 1870s for organic substances, is characterized by less rapid but more stable exponential growth without saturation until today. Significant deviations from ideal exponential growth can be explained by war effects. But, surprisingly, there are caching-up phenomena in post-war periods which cannot be explained by external factors only. A "push-and-pull" model (man-power and research activity, on the one hand, techno-economical interest, on the other) obviously fails. Instead, the exponential growth of chemical substances seems to be determined by methodical constraints. We can set up three specific methodological models for exponential growth in preparative chemistry. The models explain the preparative capacity at any time in relation to the respective amount of methodical resources on different levels: the combinatoric approach on the level of substances as tools, the analogical approach on the level of empirical recipes, and the feed back approach on the level of theoretical methods. Although a combination of all approaches is conceivable, there is some evidence (catching-up phenomena, historical continuity) that the last two have been more important at least in organic chemistry. A further scientometric study (*Schummer* 1997) will clarify this point and, moreover, settle the methodological difference between organic and inorganic chemistry which is reflected by quite different growth rates.

Notes

1. Cf., e.g., *Moravcsik* 1973, *Gilbert* 1978, *Rescher* 1978 (Sect. VI and quoted literature), *Tague* et al. 1981.
2. So did already the young *Price* (1951, p. 91): "We may therefore interpret the rate of growth as being an index of the scientific man-power mobilized around the field studied."
3. The birth and stimulus model, respectively, is from *Price* (1951, p. 91; 1961, p. 169), the epidemic model has been suggested by *Goffman & Newill* 1964 and first applied by *Goffman* 1966.

4. For a comparison of the number of abstracts in chemistry, biology and physics see *Price* 1963, p. 10 and *Tague* et al. 1981, p. 133. According to the latter the cumulative numbers of chemical and biological abstracts (1960–80) are five times and two times higher, respectively, than that of the corresponding *Science Abstracts*.
5. Cf. Chemical Abstract Service 1996; for details concerning the methods of registration see the *Registration Policy for the CAS Chemical Registry System* and *CA Index Guide,* both available at CAS.
6. For source references cf. the legend to Fig. 1.
7. For instance, the index of Beilstein's handbook does not distinguish between different poly-halogen compounds or configuration isomers with different substuent position until 1899, derivatives of carbon acids are not recorded until 1903, and cis-/trans-isomeres are not distinguished until 1929.
8. The adjustment was achieved by optimized extrapolation of the CAS data to the value of 1959 and yields a basic value of 1.76 mio for 1964, which is in agreement with estimates of CAS (1.5–2 mio, information by letter). Notice, that CAS has included some substances prior to 1965 in the registry system during the years 1973, 1985–1990, which had to be substracted before.
9. *Morveau* et al. 1787.
10. The speculative character is very obvious, for instance, in the tables of Lavoisier 1789.
11. Cf. *Mulkay, Gilbert & Woolgar* 1975 and *Edge & Mulkay* 1975 for comparative studies on such 'explorative phases'. Notice that, in contrast to their model, the explorative phase in preparative organic and inorganic chemistry show more rapid growth than the following.
12. The deviation related to the French-German war is presumably too large, because the only datum available for this period is from Richter's first edition which is expected to be of restricted scope (cf. Sect. 2).
13. *Price* 1963, p. 5; the law was already formulated in *Price* 1951 and 1956. For predecessors cf. *Rescher* 1978, p. 54f.
14. Data are mainly from *Partington* 1961–70, *Ihde* 1964 and *Brock* 1992. Notice, that *Price*'s (1963, p. 29) representation of the growth of chemical elements in the period 1730–1950 is inadequate for two reasons: (1) The modern concept of chemical element was fixed only in the late 1780s by Lavoisier's operational definition (*Schummer* 1996, Sect. 4). An 18th century chemist would have considered Price's exponential growth of elements just as an arbitrary collection of composed substances. (2) Unlike Price's incomprehensible distinction between "chemical" and "physical" elements (what makes, for instance, rare earths of the 1880s more "physical" than those discovered by similiar methods in the 1840s?), there were at least 9 relatively independent research programs (Fig. 2).
15. Notice, that after 1789 only 4 elements were discovered by chance without any connection to one of the research programs: Cd (1817, Stromeyer reduced zinc carbonates), Se (1818, Berzelius reduced selenites with SO_2), V and Ru (1830/1844, Sefström/Claus found them in Swedish ores).
16. Further instable elements predicted by Moseley (Tc, Pm, At) were artificially made later (cf. *Partington*, op. cit., vol. IV, pp. 951, 955).
17. *Rescher* 1978, p. 102; his intermediary patterns are "very important" (annual growth rate, 1.25%), "important" (a.g.r., 2.5%), "significant" (a.g.r., 3.75%).
18. Notice, that even if innovations are *slowly* exhausting (mean innovation time << mean exhausting time) a linear sequence of innovations – e.g. *Holton*'s (1962) escalation model – yields a linear growth of products. This (linear) case can easily be modelled in mathematical terms by setting up a sequence of logistic curves.
19. Data about articles and chemical patents are drawn from *CAS-Statistical Summary 1907–1995*. The number of chemists is ascertained from *Chemical Abstract, Collective Author Indexes* by random sample survey (error estimated less than 10% (α=0.05). Since the *Collective Author Indexes* cover periods of ten years before and of five years after 1956, we get two slightly different definitions of a chemist: somebody who is author or co-author of at least one chemically relevant publication within 10 (5) years. The difference disappears when mean annual productivities of substances or articles per chemist are calculated as it is done for Figs 4 and 5.
20. For details cf. *Schummer* 1996, Sect. 6.

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