THE TOP TWENTY AND THE REST: BIG CHEMISTRY AND LITTLE FUNDING

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The Editor of this annual series was generous in his invitation to me to prepare an introductory chapter. The charge was equally generous in that it permitted me either to reminisce about my career or to be philosophical about the present state of physical chemistry. The first topic could not be usefully padded to fill a chapter, and I have severe reservations about a bureaucrat pontificating about the direction in which science is going. A reading of the chapters following this one will yield a definitive statement of the present state of the science and give the reader a good signpost to the future.

Therefore, as is usual in science, I will not respond to the problem proposed, but to an easier one, one with more circumscribed boundary conditions. I will share with you my views on the support of chemical research and outline what I consider to be some current problems. This approach will differ from the usual introductory chapters in this series in that it will not be entirely factual but will include opinion. Much of what follows is based on the operation of the Chemistry Section of the National Science Foundation, but it must not be construed that the procedures described are those of all funding agencies in the United States or for all areas within the NSF. Further, in no sense should my statements be taken as the policy of the Foundation as enunciated by the National Science Board.

When one is offering opinions or exhibiting one's biases, readers should be aware of the background responsible for such viewpoints. Briefly, I did my undergraduate work at a then small, public university (Utah), graduate work at a small, private technical institute (Cal Tech), spent eight years at a major, private university (Harvard), was chairman of the department at a small, private university (Tufts) for ten years, and Head of the Chemistry Section at the National Science Foundation for eight years before moving to my present position.

It may be useful to comment on my move from the academic world to the federal bureaucracy. There are a number of reasons one might give for such a change in position. The obvious reason of realizing one can no longer compete in creative research must be discarded out-of-hand no matter how true it might be. While individuals will describe it differently, I believe most of us would agree it is the opportunity to make another contribution to the discipline that attracts us. Until I was asked to take a two-year leave from Tufts to fill the vacancy caused by the retirement of Walter Kirner, I had given no thought to government service. After being immersed in the Foundation, however, I eagerly accepted the offer of a permanent position. What follows, then, are my impressions of how one goes about doing the public's business of supporting basic research and some of the problems in that business.

I had always been aware that a very large fraction of the cantankerous scientists worked for granting agencies and was absolutely amazed to discover that when I moved to the NSF, they transferred to academic institutions. One is struck by the "we" and "they" aspects of the relationship between the working scientist and his counterpart in the agency. "We" sit between Congress and the Office of Management and Budget and the bench scientist. In a real sense our primary goal is to provide the best research people with the additional resources they need to do the most innovative research. Primarily because of lack of funds, we never achieve our goal even for a few individuals. Thus, we spend our time trying to get the best research out of our limited funds. We frequently feel that "they" sit on their hands and do little to explain to the public and, hence, Congress what basic research is and why it should be supported from the public purse. The central questions are always whether we make the best decisions on programs and on individual proposals and, on the personal side, whether our being in the funding agency has made any difference to the health of science. It is frustrating for a person trained in science to be unable to answer those questions or even to devise experiments that yield answers.

The basic decision we make, and the one the applicant feels most directly, is whether or not to fund an individual proposal. The program director is most intimately concerned with that decision. The decisions of a program director are always subject to several levels of review by section heads and division directors, but because he is the most knowledgeable person in the Foundation in the subject area of the proposal, his assessment of its scientific quality is crucial. These day-by-day decisions implement directly the policy of the National Science Board. Program directors state that theirs is the best job in the Foundation, and they know this is so because the rest of us are always trying to play program director.

Because of the position held by the program directors, it is critical that the best qualified people be attracted to these jobs. They not only have to be knowledgeable in their field of science, but they must be equally knowledgeable in the sociology of science. The chemical community was incredibly fortunate in having a person of the caliber of Walter Kirner as the first program director for chemistry in the Foundation. It is difficult to overestimate the crucial role he played in setting the intellectual tone of the Section. His education at the University of Illinois and Harvard University and his thesis work with Roger Adams (MS) and James B. Conant (PhD) gave a firm beginning to his productive career. Prior to joining the Foundation in 1952 to initiate a granting program in chemistry, he had held academic positions at Middlebury College, Rice Institute, and Carnegie Institute of Technology, had been Chief of Division Nine of the Office of Scientific Research and

Development (OSRD), and later Director of the Chemical Biological Coordination Center of the National Research Council. For his work at OSRD, he received in the same year the Presidential Medal of Merit and from Britain, the King's Medal for Service. He recognized the value of research participation by undergraduates as well as high school and college teachers. He supervised these programs until they were transferred to the Education Directorate. When chemistry within the NSF was expanded from a program to a Section in 1963, he was appointed Section Head and remained in that position until his retirement in 1965.

In the 22 years since a granting program in chemistry was established at the NSF, there have been only 22 program officers, including nine current incumbents. Because of the nature of research, it is important that the program directors dealing with research proposals not be too far away from the bench themselves. On the other hand, proficiency in dealing with the bureaucratic aspects of proposal-processing and decision-making does not automatically come with expertise. Thus, some mix of longer-term and short-term program officers is desirable. It is only recently that the Chemistry Section has had a significant number of people on leave from other institutions. A major obstacle to maintaining rotation appointments is that for the reasons mentioned before, many rotators become infatuated with bureaucracy and wish to remain. The ex-Section Head is a case in point. NSF procedures allow the permanent program directors to spend up to one day a week doing research. A number of program directors exercise this option. There is also a sabbatical program that provides for a full year of research for a few staff each year.

The decisions on research proposals will be no wiser than the people who make them. It is, therefore, in the enlightened self-interest of the research community to provide a constant stream of highly qualified people to take temporary or long-term positions at granting agencies. My experience is that the chemists in the external science community care little about this problem. I find this indifference to an important problem on the part of the research community to be appalling.

Advisory panels are an important mechanism for interaction between Foundation staff and the external scientific community. In the beginning, it was necessary to use the advisory panel for chemistry to review proposals and to make detailed funding recommendations, because even Walt Kirner did not have high expertise in all subdisciplines of chemistry. Although the chemistry staff had expanded somewhat by 1966, the advisory panel still reviewed all proposals to recommend priority and budget amounts. In 1967, after additional staff was added to the Section, it was possible to take the desirable step of ending panel review of project proposals, although panel review continued to be used for the departmental instrument proposals. After an experiment that showed that the results of panel review and ad hoc mail review were statistically highly correlated, the Section moved in 1974 to complete mail review, leaving the panel time to do what is more valuable: consider the operation of the Section in general and give advice on the future directions and needs of chemistry.

I feel that mail review is superior to panel review. While I understand that discussion in a group can often uncover and straighten out misconceptions, just as often a strong personality can dominate such discussion and negate the positive aspects of panel review. The volume of proposals that are received by the Section (1100 in 1974) is too large to be dealt with by one panel, and if one had to use several panels, much of the intercomparison obtained by panel review is lost. A more important reason, in my view, for removing the review of individual proposals from the panel is to make the position of program director more attractive. With a panel making grant recommendations, one does not need a highly trained scientific staff. The Section Head could run that part of the operation with secretaries. Since the granting mechanism is only a part (albeit major) of the activities of the Section, such an arrangement will not do. To understand the needs of the chemical community and to formulate programs responsive to those needs we must have outstanding technical people. This is particularly important in times of level funding and the attendant increased difficulty in choosing between alternative projects.

It has often been stated—and it is even true— that scientific quality is the criterion which determines eligibility for funding. The trouble with that laudable criterion is that it has poor resolution. This problem is illustrated schematically in Figure 1. With five mail reviews on each, two proposals would have to differ by one full point (VG--G, for example) to be statistically different in quality. The real situation does not approach that. We always run out of money in the middle of a group of proposals where the scientific quality is very high and the quality of individual proposals is virtually indistinguishable. Because of this low resolution of the high scientific quality of the proposals with which we deal, we are forced to use secondary criteria. We are in the position of an admissions officer who can admit 300 students but has 600 applicants with Board scores of 800. He starts looking for a left-handed shortstop or a piccolo player. Because each program director has by necessity subject

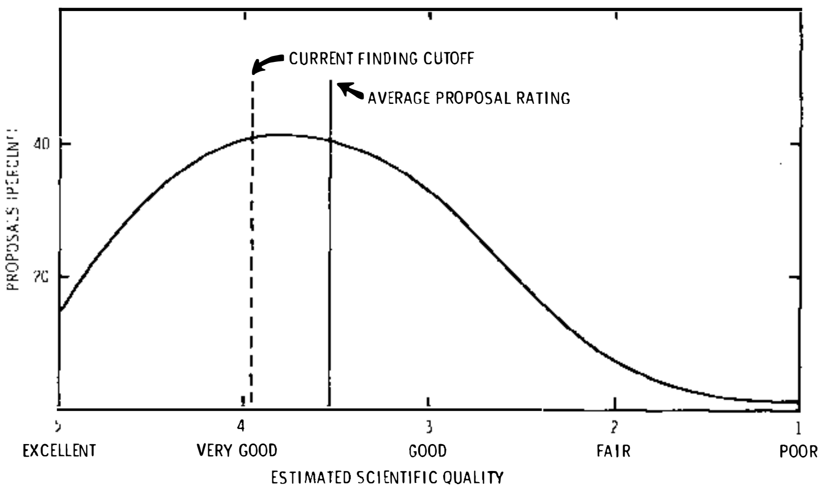

Figure 1 Quality rating distribution of research project proposals (Chemistry Section, the National Science Foundation).

matter of considerable scientific breadth under his purview, his scientific judgment becomes very important. Such judgment, like any other talent, is hard to come by and difficult to teach. Most of us lesser mortals would like to have secondary criteria with clear objectivity.

An attractive secondary criterion–in addition to adequate geographical distribution and opportunity for participation by a broad range of research performers–is the use to which the results of the work would be put. That determination is almost a reformulation of scientific quality and gives little increase in resolution. One can ask, however, the related question of how much use has been made of the investigator's previous work. With the exception of maiden races, past performance is a useful criterion at the race track. It will not predict that Upset would beat Man-O War, but it strongly implies that if you keep betting on Man-O War, you are going to cash some tickets. Of course, one also bets on first-time starters in the hope they will be winners. A similar situation exists in research.

If one assumes that a reference in a published paper is an acknowledgment that the work reported is based on, or indebted to, this prior work, it can be argued that the number of citations a publication receives is a measure of the use the scientific community makes of a given publication. Many objections can be raised to the use of citations to measure the importance of a publication, e.g. a paper that is wrong and in a hot subject will attract a large number of citations. Also we can all think of papers that were unappreciated for years before being recognized as reporting fundamental work. Yet, in spite of the obvious pitfalls, citations are on average an indication of the usefulness of a published piece of work and therefore worthy of study to see if they might be included among other secondary criteria. Of course, such numerical compilations must be used with

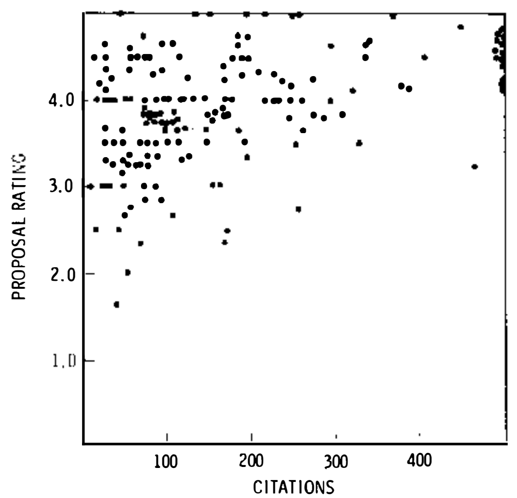

Figure 2 Quality rating of research project proposals vs citation record of the principal investigator (Chemistry Section, the National Science Foundation).

judgment. This is particularly true of citation counts since their real significance is unknown.

A number of studies (1) have been completed or are underway that attempt to assess the usefulness of citation data. The Chemistry Section did a small scale experiment involving data for the graduate faculty in the 79 chemistry departments listed in the Roose-Anderson Report (2) on graduate education. This study found, as others had in other disciplines, that a ranking of departments by the average number of citation per faculty member correlated well with rankings achieved with other data.

I believe citation data can help our decisions on individual proposals. Figure 2 is a plot of the rating of a proposal vs the total number of citations (excluding self-citations) made to the investigator's published work during a five year period. The data shown are for a particular program, but data from all chemistry programs are superposable. Also similar plots are obtained if one treats young and established investigators separately. The rating given to each proposal is the average of those assigned by the mail reviewers presumably without recourse to citation data. The correlation between proposal rating and number of citations is very low. No highly cited investigator gets a low rating on his proposal, but the reverse is not true. Many proposals which receive high marks come from investigators who publish very little and when they do publish, little attention is paid to the work as judged by the number of citations made to it. I believe this is another indication that most of us are better at promises than we are at delivering the goods. I suggest that both the reviewers and the program staff in the Chemistry Section have been putting too much emphasis on what is promised in the proposal and too little emphasis on how the investigator has produced in the past.

Many who are less optimistic than I that valid conclusions can be drawn from the number of citations to a single paper or to the work of an individual do feel that citation data can give an indication of interactions among subdisciplines or of the relative importance of a research field as a function of time. The results of the preliminary study undertaken by the Chemistry Section were sufficiently encouraging for a comprehensive investigation to be undertaken of the citations made to the papers published by the faculty of the PhD-granting chemistry departments in the United States listed in the Graduate Directory published by the American Chemical Society (3) plus a large number of selected research workers in other institutions and laboratories. I believe increasing use will be made of citations and similar data in both pre- and postgrant evaluations as the limitations and inaccuracies of such data are better understood.

Another major concern and responsibility of the Section is the allocation of resources among subdisciplines and support categories. Such allocations are influenced by the program structure one chooses. When chemistry within the NSF was expanded to a section, it was divided for administrative purposes into the traditional chemical subdisciplines: organic, inorganic, analytical, and physical. This structure existed until 1967. By that time it had long been clear that the traditional subdivisions of chemistry had little use in describing the activities of modern research chemists. With the possible exception of synthesis, the differences among the traditional subdisciplines had disappeared as mathematical and instrumental techniques spread to all branches. I find it remarkable that so few graduate departments have recognized this fact in their own internal organization.

In 1967, the Chemistry Section was reorganized into a program structure that reflected the main questions chemists ask about substances:

What is it?—Chemical Analysis and Instrumentation
What is its molecular structure?—Structural Chemistry
What are the electrons doing?—Quantum Chemistry
How is it made?—Chemical Synthesis
By what mechanisms and how fast does it react?—Chemical Dynamics
What is its bulk behavior?—Chemical Thermodynamics

To give added emphasis to the increasing importance of instrumentation, it was made a separate program in 1971. In recognition of the fact that organic and inorganic synthetic methodologies, although converging, are still somewhat different, the dichotomy that existed in the synthesis program was formally admitted in 1972 by the establishment of separate programs of Synthetic Organic and Natural Products Chemistry and Synthetic Inorganic and Organometallic Chemistry. As all questions asked about chemical systems have theoretical components, there is no separate program for chemical theory. These program titles are related to, but not identical with the categories used in the Westheimer Report (4). The Section can operate under any organizational pattern and there will always be interface problems, but I believe the existing structure is the most useful one in view of the changing directions of chemical research.

The disciplinary advisory panels continue to be a major focus for interaction between the external scientific community and the staff of the Foundation. An important duty of the panel is to advise on the allocation of resources among programs by transmitting their own as well as their colleagues' perceptions of the future trends in chemistry and its impact on allied fields. Advisory panel members are chosen by the Foundation and, although they must be appointed for a year at a time, by tradition they have had a tenure of three years. Recently this tradition has been broken, with some members asked to continue longer and others serving for shorter periods. The prime characteristic of a desirable panel member is that he combines high competence in his research field with broad understanding of both chemistry and the mechanisms of science.

Including current panelists, over the lifetime of the Foundation, 101 individuals have served the community on the advisory panel for chemistry. These individuals came from 95 academic institutions, four industrial laboratories, and two government laboratories; 48 academic institutions that offer a PhD degree in chemistry and one undergraduate college are represented. Among them, the panelists have to date collected 70 awards administered by the ACS, including nine ACS Awards in Pure Chemistry. The Section has over the years sought advice from the knowledgeable members of the profession. Efforts are also made to achieve a mix of talented young and established investigators, with as wide a geographical distribution as possible. The preponderance of academic panelists occurs because we deal overwhelmingly with academic chemists and need their view emphasized on our panel. This situation is changing and I am certain that there will be increased participation in all phases of our operation by scientists from industry, other government institutions, and not-for-profit organizations as well as by representatives from the general public. This change reflects the Foundation's growing concern for a broader participation by the community in the decisions made concerning the disbursement of public funds.

There is a formal, long range (five years) planning procedure that begins with the views of the program directors and after several cycles is modified into the overall plan of the Research Directorate. It is through interacting with the program directors in formulating these plans that the panel members have their most direct input to the allocation of funds among programs.

Although the perceptions of the panelists are important, it must be admitted that at any particular time their impact will appear small. With a level or slightly rising budget, major shifts in allocations are difficult and unlikely except under the most unusual circumstances. It would be extremely difficult to cut one program in half to double another one. By and large we practice enlightened incrementalism.

Proposal pressure is no longer, if it ever was, a useful measure of the needs and opportunities in a field. It is the product of the volume and the intellectual quality of the research ideas in a field that speak to the need for increased support. To plan effectively, the program directors must know early in the fiscal year what their budget will be. At the same time, before the fact, it is difficult to estimate the total number of high quality proposals expected in each program. The Section has approached this problem by allocating 80–90% of the available funds to programs as early in the year as the total budget is known. This allocation is based on prior commitments, expected renewals of existing grants, and new proposals on hand. The remaining funds are kept in a section reserve. At the end of the granting period, a competition internal to the Section is held for these reserve funds. The goal of this competition is that the last grant recommended in one program have the same intellectual quality as the last grant recommended in all other programs within the Section. This procedure results in moderate changes in the growth rate of the programs. On occasions it becomes obvious to a program director that he can not obligate his allocated funds without dipping below the quality cutoff in other programs. Thus, funds are transferred out of his program into another or into the section reserve. It must be admitted that the more usual situation is for a program director to determine that his quality cutoff will be astronomically high if he does not get additional money.

Recent funding history by program within the Chemistry Section is given in Table 1. Funding for projects in solid state and polymer chemistry, which now resides in the Materials Research Division, is also included. The differences in the absolute magnitude of the dollar values as well as their uneven growth reflect the above considerations.

Perhaps the most interesting aspect of the data presented in Table 1 is the difference in the total between Fiscal Years 1974 and 1975. This 35% increase from the one year to the next is almost entirely due to the perceived relevance of chemistry to energy. A major amount of that increase in funds for basic research in chemistry could be spent only for support of projects that had a clear relationship to energy. For the

Table 1 National Science Foundation research project support for chemistry (in millions of dollars)

	1970[a]	1971	1972	1973	1974	1975
Synthetic Inorganic and Organometallic Chemistry	\$1.56	\$1.75	\$2.26	\$2.32	\$2.20	\$3.40
Synthetic Organic and Natural Products Chemistry	2.49	2.67	2.81	2.82	3.14	3.60
Structural Chemistry	3.02	3.25	3.66	3.60	3.80	4.40
Quantum Chemistry	3.40	3.71	4.15	4.03	3.88	5.00
Chemical Dynamics	3.62	3.72	4.32	4.66	4.63	6.50
Chemical Thermodynamics	1.86	1.40	2.41	2.57	2.34	3.10
Chemical Analysis	1.80	1.89	2.99	2.63	2.90	4.10
Chemical Instrumentation	1.70	1.70	1.70	2.38	2.59	3.50
Solid State and Polymer Chemistry[b]		0.80	2.00	2.10	2.10	3.50
Total	\$19.45	\$20.89	\$26.30	\$27.11	\$27.58	\$37.10

[a] Fiscal Year.
[b] Division of Materials Research.

first time the Research Directorate of the Foundation had two kinds of money: one to support the best basic research proposals submitted to it and a second kind to support the best basic research proposals submitted which also appear to have a relationship to a solution of the energy problem. There are a number of chemists with impeccable research records who view this development with horror. They are certain that at last "they" have determined what "we" are and we are now just haggling about the price. I feel just as firmly that virtue is its own reward. The top 5 or 10% of the research workers in the country will always be supported at some level with public funds. This probably would be true even if they aggressively insisted that they did not care whether their work was ever useful in meeting the needs of society. However, additional funds to augment the support of the best investigators or to expand the number of investigators who receive federal funds will come only from a public that is convinced of or at least aware of the relevancy of basic research to its welfare. An essential ingredient in this conviction is clear signals from those doing basic research that they are mindful of the public needs while they are seeking to advance the frontiers of knowledge. I believe it is inevitable and also right that the appropriation of public funds for the support of basic research be tied to relevancy criteria external to science itself. I do not believe that reconciling the needs of science and the needs of the public will be easy. Indeed, I believe the establishment of this reconciliation to be the major challenge to the bureaucrats of science in the years ahead. We must capitalize on the real relevancy of basic research without trying to tell the research community what experiments to do. I know it can be done, but it will be needlessly difficult if some of our friends argue loudly and publicly that science should be supported for its own sake—like opera.

Chemistry as well as other disciplines has a guns or butter problem. It is impossible to do frontier chemical research without frontier instrumentation. Such instrumentation is expensive, but so is the support of graduate students and post-doctoral personnel. When the choice has to be made, the predilections of the chemical community, both principal investigators and program directors, is towards supporting personnel rather than buying equipment. The average dollar value of a research grant administered by the Chemistry Section has also mitigated against instrument purchases as well as inclusion of such items in research proposals. Thus, on the average the instrumentation available to even the most able investigators is rapidly becoming obsolete. Not only is it wearing out, but it is becoming noncompetitive. Rapid instrumental development and inflation has exacerbated this old problem. Kirner recognized the central position instrumentation holds in chemical research and initiated the special program for departmental research equipment. Eligibility for grants in this equipment program was based upon both the quality of the proposed research to be performed with the instrument and the number of investigators the equipment would serve. Through most of the history of the chemical instrumentation program, it was part of a line item in the Foundation's budget. To move funds between this and the rest of the programs in the Section almost literally took an Act of Congress. This situation changed in Fiscal Year 1973 when the line item for equipment was abolished and subsumed under project grant support. The Foundation, hence the Section, now has the responsibility of dividing its budget between the instrumentation program and the subject matter programs.

As I stated before, it is very recently that the advisory panel to the Section has not reviewed the instrumentation proposals. Folklore alleged that because of the diverse nature of the research described in the instrumentation proposals, panel review was indispensable. An ad hoc mail reviewer would either throw up his hands at such a complicated problem or at best only comment upon the work that impinged on his speciality. Folklore underestimated the size of the ego of the average chemist. In an experiment done last year, it was demonstrated that only 2 out of some 80 reviewers declined to review because of the complexity of the problem or other reason, and that the ranking obtained from the mail review correlated very well with the priority list produced by panel review.

Placing the departmental instrumentation program on the same review basis as the project grant programs rationalizes the allocation procedure. Now, to a first approximation, funds can be allocated to the instrument program such that the quality cutoff as judged by the same procedure is the same as the other programs. At this writing, it is too early to know the size of the allocation change this will engender, but I believe the sign of the change is clear—increased funds for equipment.

This program has been most useful to the preparative side of chemistry. By necessity most of the money has gone to purchase commercial spectrometers and chromatographs. Although it might warm his heart to know that there is the latest 100 MHz Fourier transform NMR spectrometer down the hall, the research program of a physical chemist interested in molecular beams is not helped one bit by access to this machine. More than that, it is clear that the existence of the Departmental Instrument Program has distorted the hiring policies of some departments. By having the possibility of obtaining spectroscopic instrumentation through the NSF program because of broad departmental usage, some departments have recruited in fields that were not consonant with their intellectual needs. The Section has recognized this problem and has started to fund instrumentation for individuals as well as for departments out of an expanded program. This should strike a blow for intellectual honesty. We have seen a number of proposals where a department clearly wanted the instrument for one individual, but taught five other investigators to spell ESR and submitted a joint proposal.

The unavailability of state of the art instrumentation to many excellent investigators creates another fiscal problem. It is well known that most experimental science is redone every ten years or so as new techniques or higher resolution become available. This is to be expected as it is the very nature of scientific inquiry. The current problem is a different one. Advances in instrumentation have outstripped our ability to provide this equipment to all but a few investigators. Thus, we are in the position of funding very good ideas that have to be pursued on second rate instrumentation. We know that the work probably will be repeated in the future on equipment that is in existence today. Perhaps we should only support those few leaders in research whose scientific stature provides them access to whatever they need.

Another possible solution to the problem is for the chemists to take a leaf from the book of the particle physicist or the astronomer. In both of these disciplines the time has long passed when an individual investigator or even an individual department or university could have sole title to an accelerator or a very large telescope. Chemistry, on the other hand, still operates as a cottage industry. With rapidly increasing sophistication and, hence, cost of chemical instrumentation, the chemists must face up to the question of regional or national centers as a way of life. These questions have been around for a long time, but the majority of the chemical research community has always said, "Mother, I would rather do it myself!" Although the national experience with regional centers for instrumentation for chemistry has been pretty disastrous, I feel that is because the chemists never really wanted them to work. The high energy physics model of block support for the installation, project support to user groups, and user committees to allocate instrument time certainly is applicable to other disciplines. The thorny question, other than where one locates such centers, is what instrumentation is a candidate for inclusion in a center, or phrasing it differently, where is the dollar cutoff? Although high field, Fourier transform NMR spectrometers are so expensive that not all highly innovative investigators who should have access to such a spectrometer can do so, it makes no sense to think of one instrument serving a region because it takes only a very few chemists to saturate it. This may not be true for a high resolution mass spectrometer. Perhaps the first national center for chemistry in the United States will be a computing resource.

The rationale for the centers we have been describing has been the cost of an instrumental technique. This is not the only driving force for concentrating research efforts in institutions outside the usual university structure. There is increasing questioning within the research community whether the university is the optimum location for undertaking the most creative basic research. Historically the universities have always proclaimed their mission to be both the creation and dissemination of knowledge. In a budget crunch, teaching is always protected over research in spite of the stated duality. In fact, most university administrations give the clear impression that they will tolerate research as long as it does not interfere with their business and someone else pays for it. Further, it is feared that the push by the public for immediate solutions to our pressing national concerns will make the universities inhospitable to basic research and its long term payoff.

about institutes that if their purview is too narrow, they tend to lose their vitality and their major preoccupation becomes self-preservation. With a broad charter, they are either small and diffuse or too big to be manageable. Nonetheless the question of the institutional structure which optimizes the return on the public investment in basic research is a serious one. I believe the scholars and the public must give serious thought to this and begin some experiments to determine what type of organization would be most congenial to the United States if and when it is needed.

Regardless of the institutional structure there is always the question of concentration of resources vs spreading the wealth. For a funding agency this question has two parts: the size of individual project grants and the relative concentration of funds into a given department or institution. In spite of the view held in some quarters, the program directors do not get their jollies by declining requests for support. The inclination is almost always to cut budgets to be able to fund an additional investigator. Several years ago the Chemistry Section decided that the program directors had reduced individual budgets to too low a level in trying to fund the maximum number of highly regarded proposals. A decision was made to increase the size of the average grant to give the project more than bare subsistence. This decision was taken at a time when there was no expectation that the Section's budget would be increased. Subsequent to that decision, the budget available to the Section has increased, but the decision resulted in fewer proposals being recommended for support. Is this decision, resulting in the concentration of funds, in the best interests of creative basic research?

It is true that a small percentage of the research community leads the way for the rest of us. It is equally true that past performance is one of the best clues we have as to who will make the next advance. The same analysis holds for a department. Just as we try to fund creative individuals to maximize their research efforts, should we also try to provide the best departments with the additional resources they need to maximize the collective research efforts? Table 2 displays the distribution of project support funds with the Chemistry Section to three categories of departments under the criterion that the best proposed work should be supported regardless of origin. About 15 of our list of 20 departments would appear on anyone's list and the choice of the next 5 among likely candidates does not change the statistics significantly. The group of departments called "all others" contains a mixture of historically small departments and some whose increase in size and prestige came too late to influence the Roose-Anderson rating.

The 20 departments that receive half of the public funds administered by the Chemistry Section of NSF include some of the largest chemistry departments in the United States. Although they comprise only 12% of the PhD-granting depart-

Table 2 Distribution of the National Science Foundation Chemistry Section budget among departments of chemistry

	Departmental Grouping		
Fiscal Year	Top 20[a]	Next 59[b]	All Others
1965	42[c]	45	13
1968	44	39	17
1969	40	43	17
1970	42	40	18
1971	36	44	20
1972	44	41	15
1973	49	37	14
1974	51	35	14

[a] Chemistry Section designation.
[b] Roose-Anderson listing (2).
[c] Percent of dollars obligated.

ments in the nation, they contain over 18% of the total graduate faculty and produce over 34% of the PhD's in chemistry. Because of their worldwide reputation for excellence, these departments, right from the beginning of the federal programs, have received a major share of the publicly funded fellowships and traineeships in chemistry. Thus, as other demands on the public purse have brought about severe reductions in these programs for research graduate students, the high-quality graduate programs available in these top departments have been disproportionately hard hit. I believe it is in the best interests of the United States and the health of science to see that these traditionally strong departments have every opportunity to compete effectively for scientific talent and to remain world centers for chemical research and graduate instruction. The amount of money needed beyond the project grant support received by the successful individual investigators in these departments is not large. I estimate that an increase in support of 10–15% over that currently received on research grants would go far to alleviate the problem. With a rising budget, such action could be taken without reducing the support of high-quality research at other institutions. It is interesting to note when one is considering the top chemistry departments in the country, that the large majority of them have been producing excellent research and well-trained chemists since before the federal government was a serious partner in the support of basic science. Thus, they supplied much of the base upon which has been built our present productive and widespread research enterprise.

Any opinion about the adequacy of support for a small number of departments implies opinions about the size and shape of the PhD-granting establishment. I have strong feelings about this and they can be stated very simply. There are far too many departments that offer the PhD degree in chemistry. At least half the departments will never achieve a critical mass in faculty, students, or instrumentation. In terms of both manpower training and research output, our resources are spread too thin. To maintain continuity in an experimental program there needs to be at least five graduate students. In my opinion a graduate department should have between 20 and 25 active research faculty to provide the minimum breadth of research interests and subject matter expertise. There should be 20–30 postdoctoral appointees to provide a continual influx of new experiences and points of view. Postdoctoral appointees will become more and more important as declining enrollments reduce faculty size and increase the proportion of tenured faculty. Thus, my minimum viable department has 20 graduate faculty, 130 graduate students, and 30 postdoctoral appointments. The ACS Graduate Directory (3) listed 185 departments of chemistry which in the United States in 1972 offered the PhD, with a total staff of 4,255 faculty, 13,028 graduate students, and 2,460 postdoctoral appointees. Thus, the average department is under the minimum in graduate students and postdoctoral appointees I consider viable and marginal in terms of faculty. If one calculates the research project support and capital equipment required for such an installation, one again finds a large disparity between what is required and what is available. This is another example of what Hardin described as the "tragedy of the commons" (5). There are not and never will be sufficient funds to satisfy the needs of all the able people who wish to do creative research.

I feel this conclusion very keenly as I spent ten years of my life trying to acquire the resources necessary to build and operate a PhD program. When I went to Tufts with that mandate, I submitted a cost estimate that exceeded what was actually achieved by at least a factor of two, but was certainly an order of magnitude lower than what I now realize was actually needed to achieve the goals I had established. Although I did not believe it at the time and probably would not believe it now if I were still chairman of such a department, the establishment or continuation of a PhD program with less than marginal resources is a mistake.

Although I am convinced the graduate establishment has been overbuilt, I am less certain about the production of persons with graduate degrees in chemistry. One always assumed that if one wished to spend the time and energy to achieve a PhD degree in chemistry that one was assured a satisfying and well-paying job for life. When I entered college to study chemistry, it never occurred to me to ask what the job prospects would be eight years from then. If I had asked, I am sure the answer would have been that the prospects were unlimited. This view of the situation existed until recently.

Another difference between the old days and now is the previous lack of appreciable support for research and science education. Graduate students were supported by teaching assistantships or not at all and what research support there was came from private donors or university funds. Thus, deciding how many chemists (scientists) should be trained was not, to first order, a public question. Now that the expanded academic science establishment is almost entirely dependent upon public funds, it is of public concern to question manpower production. Having concluded that manpower production is a public and therefore bureaucratic concern, how does one go about determining the need or, more properly, the amount of public funds that should be allocated towards satisfying the need? Cartter (6) showed long ago that the need for academic staff could be predicted because student populations could be predicted with some certainty. No comparable model has been developed for the industrial and government sectors. This lack is particularly troublesome for chemistry because the majority of chemists always found employment in industry. The advent of public concern for the environment and now the energy crisis have further eroded the validity of previous chemical manpower projections.

We do know, as illustrated in Figure 3, that the number of persons receiving a PhD degree in chemistry peaked in 1970 and has been dropping ever since. In a technological society the need for technically trained manpower can only increase. Even the flower children have abandoned the back-to-nature communes. I believe, but cannot prove, that we will need and use all the scientifically trained minds we can lay our hands on. At the same time we are in an era of current employment problems and the wrong-headed perceptions of many students that challenges and opportunities for service to the public are greater outside the hard sciences. Surely now is not the time to depress any further the pool of scientifically trained manpower.

My comments so far have had to do with the making of research grants and efforts to improve those decisions. These activities are similar to the administrative and research duties of academic personnel. The third aspect of academic life—teaching—also has a parallel in the federal agencies. We spend much of our time in committee meetings, making site visits, writing staff papers, and similar activities that do not bear directly on the granting business. Much of this is closely related to teaching in that we are trying to transmit our understanding of the needs and opportunities of the chemical community to nonchemists in the Research Directorate, on the National Science Board, or in the Office of Management and Budget (OMB). Similarly, we spend much time preparing textbooks (budget books) for OMB and Congress and lectures for the Director or Assistant Directors to deliver at various Congressional committee meetings.

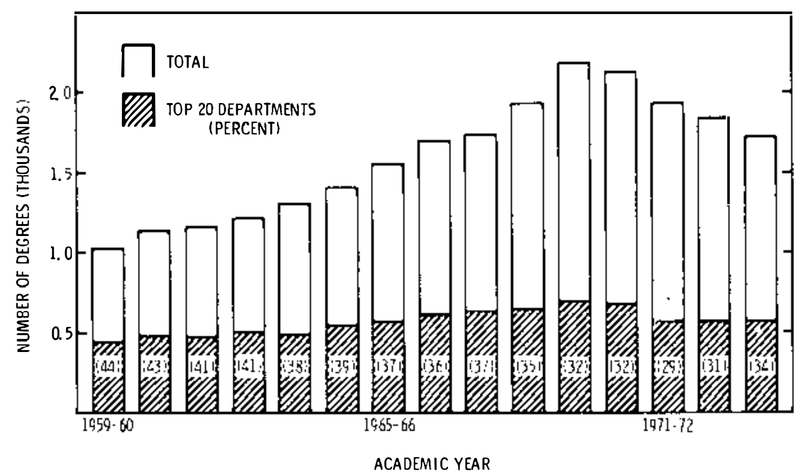

Figure 3 Production of PhD degrees in the United States (ACS Directory of Graduate Research).

We are always involved in dealing with three budgets at any given time: one that has been appropriated by Congress and we are spending, one that has been requested and is being defended before Congress, and one for the fiscal year two years ahead for which the budget book is in preliminary draft. This budget sequence is one reason why program changes are slow. The results of bureaucratic research cannot get into the budget textbook until two years after the results are known. This time lag makes it doubly important that bureaucratic planning be done thoughtfully and with the closest possible coupling to the needs of science as seen by the bench scientist. There is a tendency on the part of the bureaucrat to resent the time these teaching duties take away from making grants. Yet without succcss in this teaching, there would be no money to disburse and no need to worry about the quality of the decisions.

I began these remarks by pointing out that although they are based upon my experiences in the Chemistry Section of the National Science Foundation, they are not a statement of Foundation policy nor are they necessarily typical of any agency with which a research investigator deals, as the Chemistry Section of the NSF supplies only somewhat over one third of the federal funds supporting research in academic departments of chemistry. This underscores the last point I wish to make concerning the support of research. One must resist very strongly all attempts to concentrate in one agency funds for the support of research within a single discipline. No matter how wise a program director or the rcviewcrs he selects, thcrc always must be another jury before which the investigator can present his ideas and research plans. Just as I am convinced that it is a mistake to spread limited research funds thinly over a large number of consumers, I am equally convinced that it would be a mistake to concentrate the power to disburse public funds for research in a single agency. Furthermore, I am firmly convinced that such funds will be more wisely spent if scientists on the receiving end will learn about funding procedures and lend a sabbatical hand to the disbursing activities.

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