SCIENCE

26 December 1969

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AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE

Scientist or statistician? Some new computer developments are changing things for the better

To the laboratory scientist, the promise of the computer is relief from a growing burden of rather boring statistical work. He is much less interested in the computer's nanosecond-speed and the bit and word-size of its memory than in its ability to accumulate data, plot graphs, make long calculations and generally perform the non-creative tasks that increasingly are reducing his effectiveness as a scientist.

Given the chance, the computer can live up to its promise. But in all too many laboratories, the computer doesn't even stand the chance of a trial because it creates new problems that some scientists consider to be worse than the old. Chief among these is the complexity of putting the computer to work in the laboratory—programming it, mastering the instrument-computer and the man-machine interfaces—which, to the scientist, is often a greater drudgery than the manual data gathering and calculations that the computer eliminates.

Two more or less recent advances in technology will make the computer more readily acceptable to the reticent scientist. The first is the small, instrument-oriented digital computer, a relatively low-cost ($10,000-$20,000) machine with easy-to-use controls, often pre-programmed to do a specific job . . . as in the lunar sample analysis experiment described later. Second is the growing popularity, at lower and lower cost, of shared-time computer leasing, which reduces the physical presence of the computer in the lab to nothing more complex than a typewriter-like keyboard. When coupled with the availability of packaged programs developed by instrument manufacturers for a specific analytical purpose—as in the simulated distillation article described next—shared-time computers will satisfy increasingly larger numbers of scientists.

In both cases, the scientist can capture the advantage of the computer without suffering its complications. Use of the computer requires nothing more complex than answering a computer-initiated dialogue in English and mathematical terms that are already familiar to the analytical technique in question . . . and entering the answer on a keyboard that requires no more than a "hunt and peck" typing skill.

Shared-Time Computer Helps GC Simulate Distillation

A far cry from the alembic used by the 16th century alchemist, the artful glassware used by the modern oil chemist for True Boiling Point (TBP) distillation nevertheless employs the same basic technique: boil and condense. To this day, TBP distillation remains the only accepted way to establish the basic marketing specification of petroleum products . . . and it leaves a lot to be desired. Those who refine petroleum products don't like it because it takes so long: TBP distillation of a wide-boiling distillate can take as long as 100 hours, and the results are useless in controlling the operation of a refinery. Those who buy petroleum products don't like it because the method is not very reproducible, especially as it applies to the initial and final boiling points. Those who perform the distillation don't like it for both of these reasons and because the procedure itself is a long and boring task.

A group of scientists at HP's Avondale Division have devised a completely automatic method that employs gas chromatography (GC) to simulate distillation and produces boiling point distribution data more precisely and in much less time—about 10 minutes—than TBP distillation. The new method employs the HP 7600A Chromatograph System which is capable of automatic unattended operation from sample measurement and injection through GC analysis and digital readout of integration data.

The recipe for simulated distillation with the 7600A is relatively simple. After installing a non-polar column of limited efficiency (most of the methyl-silane silicone rubber phases are satisfactory), set the GC for a linear program of 6 to 10°C/minute starting at −20°C, load the sample tray with as many as 36 different calibration and analytical samples, even of widely diverse boiling ranges up to 1000°F . . . and push the *start* button: the rest is automatic.

The 7600A automatically injects the samples and prepares a punched tape record of the GC retention time and area measurements at precise time intervals. Complete sets of programs provided with the 7600A enable any of the principal time-sharing computer services (including the HP 2000A Time-Shared System) to read the punched tape data, determine the initial and final boiling points of each sample, assign boiling temperatures to each data point and print out the analysis report of boiling point distribution of each sample at 1% increments.

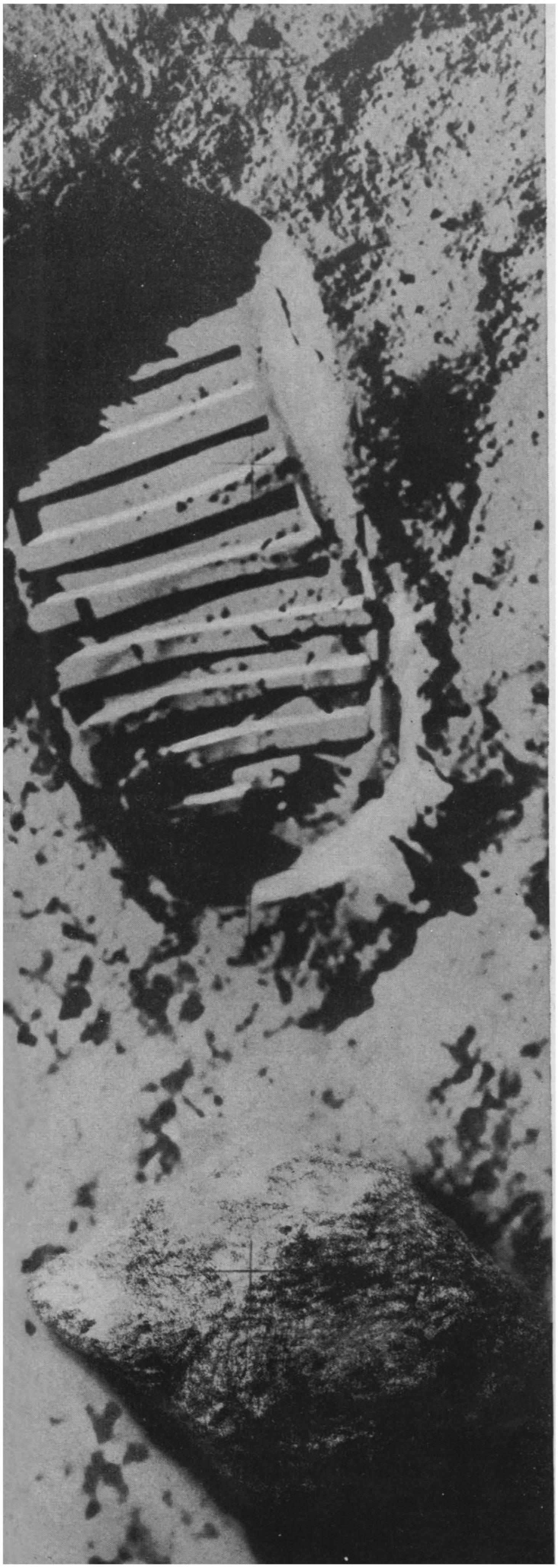
No knowledge of computer programming is required by the analyst. At each stage of the computer-performed calculations, the computer asks for the information it requires and the operator answers by typing the requested number or word on the time-share terminal keyboard.

The precision of the 7600A Simulated Distillation method with wide boiling range samples is greater than is possible by any distillation method. Its speed—an average of 10 minutes per sample—completely outclasses distillation methods.

This new automated Simulated Distillation method is examined in much more meaningful detail in Vol. 2, No. 3 of *Analytical Advances*. Request your copy today.

Dedicated Computer Extracts hidden information from Lunar sample

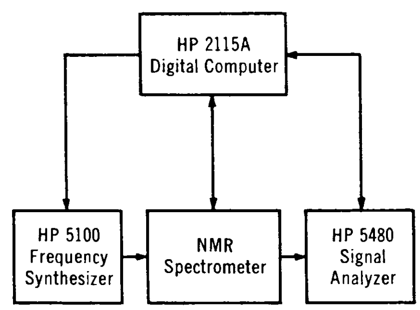
Some of the most respected scientific teams in the U.S. and eight foreign countries are performing analytical investigations on the lunar material returned to earth by the Apollo 11 crew. Among the 100-odd investigations scheduled by NASA, a nuclear magnetic resonance (NMR) analysis will be conducted by a Jet Propulsion Laboratory team headed by Dr. S. L. Manatt. Its goal is to characterize hydrogen nuclei in lunar material and attempt to establish whether any of it can be traced to free or crystalline water molecules presently on the moon's surface. The JPL scientists will also be on the lookout for heavy hydrogen whose presence will allow some conclusions about the history of the moon's surface and about the effect of the solar wind. A study



of oxygen-17 may give them important clues about the current chemical environment of the moon (from surface samples) and about the presence of a lunar sea or ocean in the distant past (from core samples).

Present-day commercial NMR spectrometers are capable of accomplishing, unaided, the work assigned to the JPL team with a creditable degree of success. But when you're analyzing samples that cost about a million dollars a gram to acquire, you're not satisfied with anything short of the best possible performance from your analytical instruments.

In the JPL team's quest for enhancing NMR sensitivity, they devised a system that combines the NMR spectrometer with a frequency synthesizer and signal analyzer under the control of a small digital computer, the HP 2115A, dedicated to this task alone.



The computer-controlled system extracts very weak NMR signals from heavy noise, enhancing instrument sensitivity as much as 100 times. It also performs fast Fourier Transforms of the NMR signal, converting it from time to frequency domain, for a further increase in sensitivity of another order of magnitude.

Here's how it works: the computer digitally sweeps both the frequency synthesizer and signal analyzer through programmed frequencies. Synthesizer output excites the NMR spectrometer which develops noise-covered resonance spikes for each nucleus in the lunar sample; under computer control, the frequency synthesizer also shifts NMR excitation between the resonance and transition frequencies of the nucleus under observation, thereby permitting measurement of relaxation or resonance decay times. The NMR output signal is fed to the signal analyzer which extracts the data from the noise and presents a calibrated display of the average signal at all times. The computer then processes the waveform, converts it from time to frequency domain by Fourier transformation and displays the result immediately in analog as well as digital form. End results of computer-controlled signal averaging and Fourier Transform is to increase spectrometer sensitivity as much as a thousand-fold. (Photo courtesy of NASA.)

Detailed information on HP Signal Analyzers and Computers is available on request. Write to Hewlett-Packard, 1507 Page Mill Road, Palo Alto, California 94304. In Europe: 1217 Meyrin-Geneva, Switzerland.

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ANALYTICAL INSTRUMENTS

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AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE

COVER

Northern elephant seal bull emitting the stereotyped vocalization which functions as a threat to other males. See page 1654. [A. L. Lowry, University of California, Santa Cruz]

WANG 700

Calculator or computer?

It's compact enough to be a calculator, thanks to the most advanced integrated circuit technology. But who ever heard of a calculator with 960 step programming capability? Or one with an 8192-bit magnetic core memory organized as 120 data registers, each of which can add, subtract, multiply and divide like 120 individual calculators? The 700 is very computer-like in its ability to loop, branch, do subroutines and make decisions. But unlike most computers, you don't have to wait to get on-line and you don't have to know a special language to use it. You'll get calculator-like convenience from its instantaneous dual NIXIE® display for both X and Y registers and computer-like efficiency from an optional automatic typewriter. You can use the 700 to conquer large and small numbers from 10^{+98} to 10^{-100}, to invert a 10 × 10 matrix, or to perform special functions like bond yields, life expectancy, nuclear half-life, or process formulas. It will execute + and − functions in 300 μsec, × and ÷ in 3 to 5 msec. $\mathrm{Log}_e{}^X$ and e^x in 17 to 35 msec and trig functions in 250 msec. The 700 can give you the right answer to a complex statistical, financial, or scientific problem before an ordinary calculator understands it or a full-scale computer is even aware of it. To simplify matters we're calling the 700 an electronic calculator, because who ever heard of a computer for $4900?*

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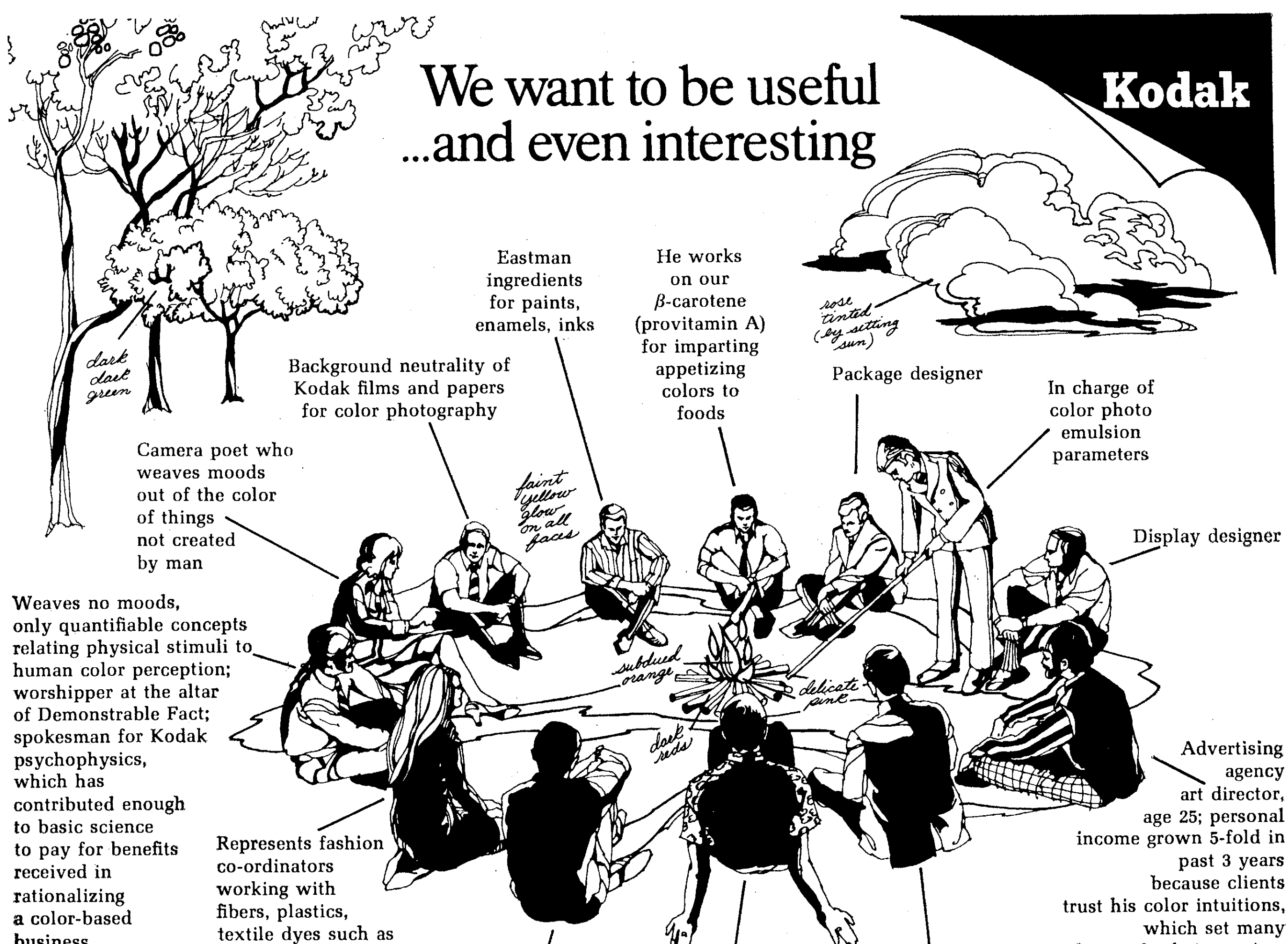
Kodak



Colorful group

We take counsel in preparation for the annual meeting of the 29-member Inter-Society Color Council in New York on April 13 and 14. ISCC, founded in 1931, brings together principal societies interested in the optics, chemistry, and psychology of color with associations of professionals in the *use* of color. For particulars, address ISCC's Secretary, Ralph M. Evans, whose address is Photographic Technology Division, Eastman Kodak Company, Rochester, N.Y. 14650.

NOTICE

All who want the newly effective EASTMAN Organic Chemicals List No. 45 but have failed to receive a copy are asked to make their need known to Eastman Kodak Company, Dept. 454, Rochester, N.Y. 14650. This one is yellow, red, and black on the cover.

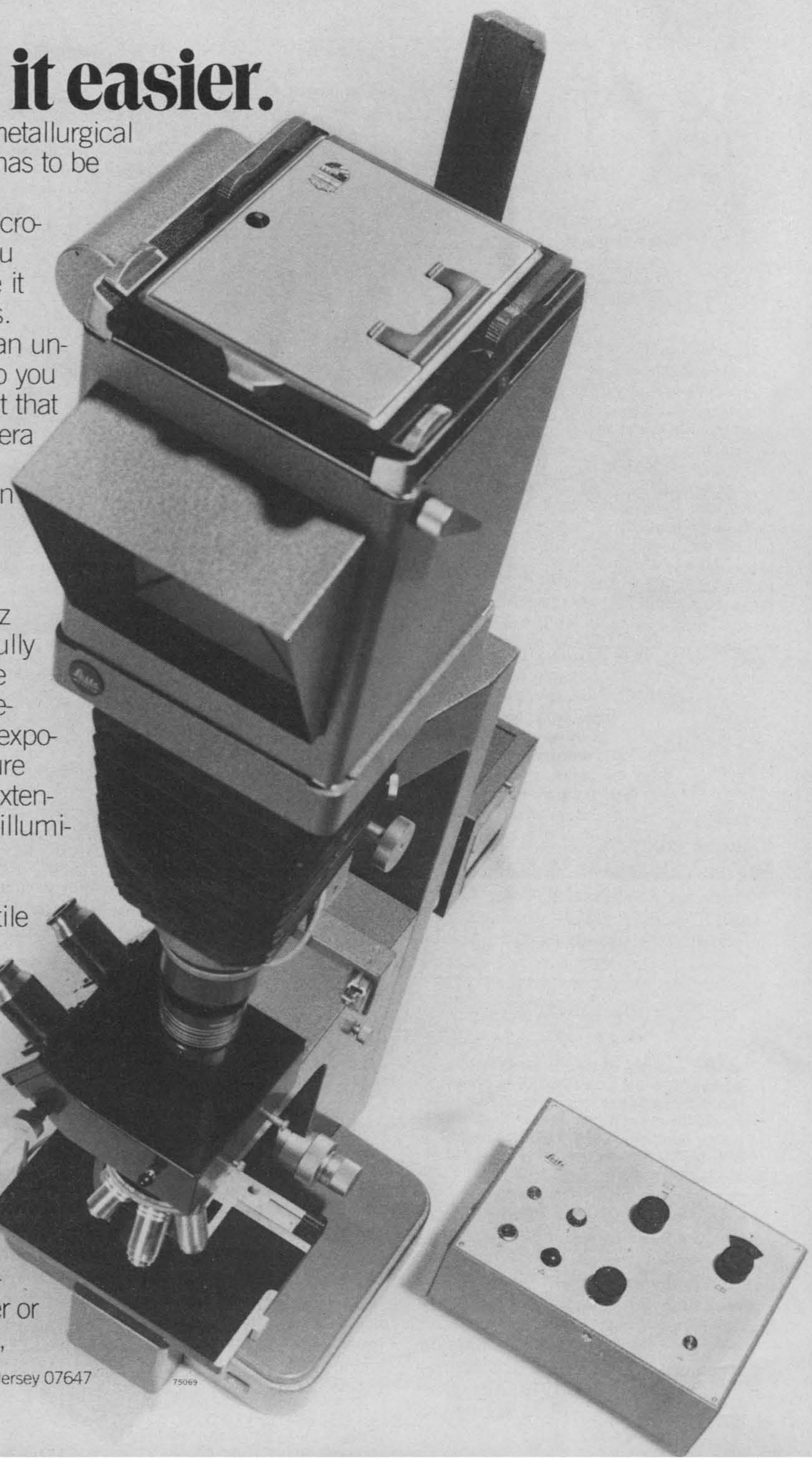
The question, after 44 catalogs since 1919, was how to continue to deserve the favor of the user of laboratory chemicals by making List No. 45 more useful than its predecessors and contemporaries.

Not only the faces on both sides of the counter but the nature of the business has changed since 1919. An alphabetical list of all EASTMAN Organic Chemicals is deemed still necessary but far from sufficient. The list is now too blamed long, and is going to get longer.

Back in 1919 a list of 100 organic compounds—all actually *available*—was beautiful to contemplate and no chore to explore, possibly even to memorize. If we could offer a hundred, why not a thousand? After a while the list did grow to 1,000. Then 3,000, then 5,000, then—whoa! Truth dawns in a new shape. At some point in the half-century, the number of attainable configurations of the familiar atoms into molecules outgrew their prospects for serving the needs of man, material or otherwise.

Finding what's wanted in a list of the present size can become a challenge, particularly if either of the parties on the two sides of the counter are less than certain what the other would call it. *Chemical Abstracts* nomenclature we have not abandoned, even while switching to the assumption that compounds which have acquired less formalistic names will be sought under those names first. Another new assumption accounts for a substantial portion of List No. 45: that 100 items or fewer sharing some structure or use make the handiest listings.

What's more, List No. 45 is easier on the eyes typographically.



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Advocates and Opponents of Medical Research

For harassed federal science administrators, this year has been wearing. Contributing heavily to their problems have been the continuing uncertainties of their budgets. No Congress has been so slow to act. The National Institutes of Health (NIH) will learn in 1970 what it can spend in the fiscal year that began 1 July 1969.

The budget-making process for NIH is more simple than for some other agencies; a review illustrates problems and permits identification of friends and foes. Significant is the emergence of Senator Magnuson (D–Wash.) as an effective advocate of NIH (he has been a long-time supporter of science) and the identification of the Bureau of the Budget (BOB) as an opponent of medical research.

Work on the fiscal year 1970 budget began at NIH in the summer of 1968 and continued through that autumn. The proposed budget was then worked over by the BOB, an arm of the President. After Richard Nixon was inaugurated, the BOB made a further revision recommending that funds for research be cut $100 million below the sums appropriated for fiscal 1969. After a fight in which Secretary of Health, Education and Welfare Robert Finch backed NIH, the President recommended that the sum of $1065 million be appropriated for the intramural and extramural research programs, a cut of $43 million below the Johnson budget. The House Appropriations Subcommittee* held hearings in March 1969. The subcommittee, chaired by Representative Flood (D–Pa.), includes no member vigorously in favor of medical research. The Appropriations Committee did not cut the budget further, however, but went along with the Nixon recommendation. The House acted in July 1969.

On 1 July 1969, with appropriation action incomplete, the new fiscal year began. The Nixon administration was under pressure to hold down expenditures. The BOB apportioned tentative cuts in spending to the various departments, including Health, Education and Welfare. In turn, Secretary Finch instructed NIH to hold overall expenditures to about 90 percent of amounts spent the preceding year. At the same time, NIH was expected to spend more for training of health manpower, and the extra funds could come only from a deeper reduction in research funds. Faced with uncertainties in the budget, NIH informed some investigators that their funds would be cut by 20 percent. Many who submitted new applications received nothing.

The relevant Senate subcommittee† held hearings in October 1969. The atmosphere was friendly. As chairman, Senator Magnuson encouraged participation of other members of his subcommittee, and Senator Cotton (R–N.H.), the ranking minority member, was also helpful. As a result, the Senate bill called for substantial (about 10 percent) increases over amounts recommended by President Nixon and passed by the House. A House-Senate conference agreed on a sum that is about 5 percent above that originally recommended to Congress.

Even after an appropriations bill is signed by the President, funds are not spendable. Some time in 1970, the BOB will tell NIH what expenditures are permitted for a fiscal year that began more than 6 months earlier. The BOB has the power to thwart the will of Congress, and it may do so. If scientists wish to comment on support of medical research, they should address their letters of praise to Senator Magnuson and their complaints to President Nixon.—PHILIP H. ABELSON

* Members of the House Appropriations Subcommittee on Labor, Health, Education and Welfare are Daniel J. Flood (chairman), William H. Natcher, Neal Smith, W. R. Hull, Bob Casey, Robert H. Michel, Garner E. Shriver, and Charlotte Reid.

† Members of the Senate Appropriations Subcommittee on Departments of Labor and Health, Education and Welfare and Related Agencies are Warren G. Magnuson (chairman), Richard B. Russell, John Stennis, Alan Bible, Robert C. Byrd, Spessard L. Holland, Norris Cotton, Clifford P. Case, Hiram L. Fong, and J. Caleb Boggs.