The Evaluator Versus the Chemical Literature*

W. H. EVANS and DAVID GARVIN
National Bureau of Standards, Washington, D.C. 20234

Received January 19, 1970

The presentation of quantitative experimental results is discussed from the viewpoint of the evaluator of data. The principal needs are a detailed description of the experimentation and numerical results suitable for reanalysis. Suggestions are made for the improvement of the content of chemical papers and the retrieval of the results. Content may be improved by preparing guides that state the minimum acceptable detail for various types of measurements. Retrieval may be enhanced by judicious editing of titles and abstracts.

One of the products of chemical research, as reported in the literature, is numerical data. In some cases these data are a by-product of the investigation, in others they are the aim of the work. In all cases, they are the source material for developing values for physical properties of substances, values which are of wide theoretical and practical use.

The evaluator extracts these quantitative data, correlates them with the existing body of knowledge, and provides the results of this analysis to scientific and technological communities.

Professional data evaluators form a small subset of the chemical population. Their working procedure is to codify and intercompare measurements of the same or related properties. They select data suitable for reanalysis, combine them, and synthesize reliable values for physical properties of materials.

The reliability of published reports of research is of major concern to the evaluator. He becomes familiar with the strong and weak points of the chemical paper. Naturally he is in favor of improvement over any status quo. This paper describes the needs of the evaluator of quantitative chemical data and offers several suggestions for the improvement of our archives of chemical knowledge—the published research articles.

NEEDS

Data evaluators are students of chemical research, not readers of chemical papers. A paper satisfies their desires if the experimental work is described well and the quantitative results are presented in a form that will permit them to be reworked. Typical notices to authors explain these points clearly.

"Since experimental results, if carefully obtained, are of long range value, they should be presented clearly and carefully.... It is especially desirable that the description of experimental work be given accurately and in sufficient detail that reproduction of results in other laboratories is possible."[1]

"The data should be presented with such precision that information may easily be obtained from the paper within the stated limits of uncertainty of the experimental background. For most studies a tabular or mathematical description is preferred to the use of graphical representation. Graphical depiction should be used primarily to portray the effect of the independent variables upon the behavior.... When data points are shown on graphs they should be unsmoothed so as not to give a false impression of experimental accuracy and curve fit."[2]

"All nomenclature should be consistent, clear and unambiguous..."[1] "...formulas for all but very well known substances should be given at least once in a paper."[1] "Use consistent dimensions and give units for all terms employed."[2]

These quotations from instructions to authors summarize the needs of *any* student of quantitative data.

To ask, in this manner, for a complete, well organized report is to make the classical demands upon an author. It is appropriate to explain why these demands remain valid.

The *description of the experimental method* is important for the very subjective process of selecting data sets that are suitable for reinterpretation. A question often asked is "Did the authors pay attention to the details that I now know to be important?" Hindsight is a powerful weapon of criticism. One paper is compared against another. If author A reports on the effects of X and Y on a property and author B reports on Y and Z, did author A know about Z? Often there is no answer available, A is silent. Of course, he cannot be faulted if the effect of Z was discovered later. However the evaluator must ask "Could it have influenced the results?"

Some common items needed in the exposition of the experimental method are:

*Based on a paper presented before the Division of Chemical Literature, Symposium on Who Reads the Chemical Literature and for What Purposes, 158th Meeting, ACS, New York, N. Y., September 1969.

Description of apparatus with dimensions (either directly or by reference to earlier work).

Calibration of equipment, including a discussion of the magnitudes of possible systematic biases for which corrections were not made.

Experimental procedure.

Environmental conditions.

Identification of analytical methods used (and proof of them if novel).

Purity of materials and how determined.

Statement of sensitivity or resolution.

Explanation of the method used to reduce the data.

Assumptions made in deriving the results.

Auxiliary data used including explicit statement of their values.

Numerical factors that relate the units used in reporting the data to the fundamental units of measure.

Reports on negative results.

If the experimental method appears to be reasonable, the data may be accepted for reanalysis. Assuming, of course, that they can be found.

The *presentation of numerical data* is a topic that has exercised many authors and editors. The evaluator, the ultimate user, ought to have a say. He needs tables of unsmoothed, raw data. Why? The evaluator's task is reanalysis. The numbers themselves will be used as input. (Graphs showing the same data are a poor second choice. They may be decoded, but only with substantial additional work and always with some loss in precision.)

In this context, what are raw data? We do not mean the original numbers read from meters, but data reported in a form that does not depend upon the interpretation made in the paper, still showing the experimental scatter, and with as little dependence as possible upon theoretical assumptions. Often these data are only one stage behind the final mathematical function presented by the author. In the last analysis, the author is in the best position to know to what extent instrumental parameters or outputs require interpretation. We need his help. We hope that he will draw the line reasonably early in the reduction of his data.

Three (extreme) types of evaluations illustrate why raw data are desirable. In the first, there are replicate measurements (from several laboratories) of the same quantity over the same range of independent variables. A knowledge of the data scatter is needed to determine the compatibility of the sets used.

A second case is more common. A property has been measured in several nonoverlapping ranges of the independent variables. The problem is to determine whether or not the data sets may be joined in a reasonable manner to yield an expression for the property which will be valid over a wide range of the independent variables. The choice of a functional form and the assessment of its suitability depend heavily upon evidence concerning the precision of the original data. The evaluator should not accept without question that functional relationship that best proved the author's point. Instead he should look for unsuspected trends.

The third case almost invariably requires that the data be recast. They are used for purposes other than those the author had in view, hence the need for interpretation-free data. The data are combined with other types of measurements and used to interrelate two properties. A simple example is the combination of rate and equilibrium data to yield another rate constant.

That the experimental results, if carefully obtained, may have long-term value is an article of scientific faith. The evaluator's comment is that the data are usually the only part of a paper that remains viable after 20 years. The interpretation may be overthrown by later work (and often is) while the data remain useful.

EXPERIENCE WITH THE CHEMICAL LITERATURE

If, as a casual perusal of guides to authors indicates, the chemical journals hope to give the evaluator exactly what he desires, it is pertinent to ask "Do they succeed?" Or, better, "How well is the chemical community meeting these standards?" All of us are responsible; we police our own journals.

The journals are, on balance, doing very well. Experimental procedures are described in reasonable detail. Quantitative data are presented carefully. The use of tables and figures is growing. Many papers are carefully organized and even readable. There has been a distinct improvement in recent years in the reporting of physical measurements even though the pressure to be brief is intense. The editors may congratulate themselves. (One may suspect that the imposition of page charges has contributed. Now that the author pays he feels freer to expand on his work.) A current sour note is the photoreduction of computer printouts as tables. Often they cannot be deciphered. Undoubtedly, the quality of the original is poor. The reproductions probably will not survive microfilming. Technical solutions are available. The simplest is to require that a deck of cards accompany the printout so that the editor may "reprint" the material.

Perhaps this claim that the journals are doing quite well is surprising. All of us can cite examples to the contrary. These counterexamples stay in mind. Some are valid complaints about sloppy reporting. But many others are unfair criticism. These include subtle problems that become evident only during careful reexamination and omissions that become significant only in the light of later work.

SUGGESTIONS FOR IMPROVEMENT

The claim in the preceding section that the chemical literature is in reasonable shape does not mean that there is no room for improvement. Careful quality control is especially important when, as is now the case, the number of chemical papers published per year is increasing. It must be kept in mind that the increase of the chemical literature is paralleled by a growth in the number of chemists. The average number of papers published by a scientist in his lifetime is between two and three. The increase in published articles means more authors, not more experienced authors.

We suggest that improved techniques for quality control are desirable. Some techniques are described below. They are applicable, now, to the present publication process.

Content of Papers. General guidance such as is given in instructions to authors is not sufficient. Specific recommendations on the presentation of data are in order. These

should tell the author what should be included in a paper on a particular subject. In the hands of a referee, they become minimum standards for publication.

The idea is not new. Minimum standards have been developed by various groups for the presentation of infrared spectra,[3,4] crystallographic data,[5,6] calorimetry,[7,8] rates of chemical reactions,[9] thermal conductivity,[10] gas chromatography,[11] measures of precision and accuracy,[12] differential thermal analysis,[13] and optical spectra.[14,15,16]

Some of these are incorporated in "instructions to authors" in various journals published by the American Chemical Society.

We suggest that there should be many more of these specific guidelines. An attempt should be made to cover each of the types of experimentation currently in vogue that leads to quantitative data.

These guide lines should be provided not only to authors but also to referees. The latter are the essential quality controllers. The referee would be asked to make sure that the paper included the material specified in the appropriate guideline. A "Manual for Referees," a collection of these guides, could accompany each paper sent out for review.

The development of these notes and the manual is a task that could be undertaken by the Division of Chemical Literature. It would encourage the division most concerned with a particular type of experiment to write the specification.

An important feature of this plan is that it may be tested. The existing literature could be examined to see whether or not the standards mentioned above have had a beneficial effect, and if they have not, why they have failed.

Retrieval. The data must be found before they can be evaluated. An organized continuing program uses two techniques: examination, article by article, of high-yield journals, and secondary sources such as abstracts, indexes, and current awareness services. The former is time consuming. Two data centers at NBS find it necessary to examine 50 journals cover to cover. This do-it-yourself indexing should be suppressed.

The answer is an improvement in the physical property indexing by the abstracting services. It is difficult to see how they can provide the level of indexing needed *on the basis of current information* without undertaking a detailed examination of each paper.

We suggest that the most profitable way to improve this indexing is by providing better information in the titles and abstracts of papers. This is a task that can be solved through a joint attack by authors and editors.

The steps are easy ones: make titles more specific and abstracts more inclusive. Why single them out for attention? Titles are now used widely in current-awareness services. Abstracts written by authors are now being used in Chemical Abstracts almost verbatim. They are the primary basis for indexing. Together they will probably be the input material used by automatic indexing techniques when these achieve the reliability demanded by chemists. Even now the automatic techniques are nearly sufficient for producing rough indexes that can be supplemented and edited by humans. It is likely that within five years the indexers will admit that the published indexes are largely machine produced. For these new techniques to be successful the input must be superlative. We can start now to put our house in order.

Some examples of emendation of recent titles follow. The additional material is in square brackets. (A pertinent comment on titles was made in the discussion at the symposium: every word in a title should carry information. Noise phrases such as "preliminary report" or "an investigation of " should be suppressed. We agree. A telegraphic style is desirable, provided that the syntax is not lost.)

The FCl_2 Cation. [Preparation and Properties of FCl_2AsF_6 and FCl_2BF_4].

[Molar Refractivity of Transition Metal Fluoride Complexes.] Comments on [an] article by R. A. Penneman [*Inorg. Chem.* 8, 1379 (1969)].

The Effect of High Pressure in the Vibrational Spectra of Square-planar Coordination Complexes [of Pt(II) and Palladium(II)].

The [Mechanism of the] Base Hydrolysis of *trans*-Chlorohydroxo-bis-(ethylenediamine)-cobalt(III) Cations.

[The Theory of] Light Scattering from Multicomponent Fluids. [Angular dependence of the spectrum.]

Dynamics of the Reactions of N_2^+ with CH_4 and CD_4. [Scattering of N_2^+, N_2H^+ and N_2D^+.]

Proton Hyperfine Splittings in the Electron Spin Resonance Spectra of [Planar Fused Ring Aromatic] Hydrocarbon Ions: ....

Anisotropy of Molecular Rotations [in Piperazine] Measured by N[uclear] Q[uadropole] R[esonance] Relaxation.

Abstracts also are easy to improve. The test is that an abstract should be complete, it should stand independent of the paper (and the title), and it should mention all *types* of measurements made, substances studied, and results obtained.

A "before and after" example follows.

> A method of measuring rate constants for the reactions of atomic oxygen (O^3P) with organic compounds is described, and rate constants are reported for the reactions of atomic oxygen with 12 chloroalkanes and bromoalkanes from 336° to 622° K.

> A mass spectrometric method of measuring rate constants for the reaction of atomic oxygen (O^3P) with organic compounds is described. Rate constants are reported for the reaction O + RHX = OH + RX between 336 and 622 K for the chloro- and bromoalkanes RHX = CH_3Cl, CH_3Br, C_2H_5Cl, C_2H_5Br, i-C_3H_7Cl, i-C_3H_7Br, n-C_4H_9Br, sec-C_4H_9Cl, i-C_4H_9Cl, i-C_4H_9Br, t-C_4H_9Cl, $(CH_3)_3CCH_2Cl$.

These are simple changes. Titles and abstracts that need improvement are easy to spot. How to effect the changes is the problem. Titles and abstracts need to be treated separately, although the impetus for change in both cases will come from the same source—the first serious reader, the referee.

A title is the property of the author. He may be encouraged to be more specific by appealing to his vanity; a general title may mean that his work will be missed by potential readers.

In contrast, it is our opinion that the abstract is the property of the editor. We propose the following rule: the editor, on the advice of the referee, may, without recourse to the author, add factual material to an abstract.

Probably editors have this power. If so, authors should be made aware of it.

A corollary of these proposals is that current restrictions on the length of abstracts must be relaxed. The abstract should be long enough to summarize both the experimental work and the interpretation. If anything must be slighted it should be the latter. (There is some evidence that there has been a *de facto* relaxation of length restrictions. What is needed is a formal statement that will encourage authors to write more precise, complete abstracts.) A longer abstract is a small price to pay for a better interchange of information.

LITERATURE CITED

(1) *Inorg. Chem.* **8**, 11A (1969).
(2) "Guide for Authors," *J. Chem. Eng. Data*, ACS Publications, Washington, D. C., 1969.
(3) Coblentz Society Board of Managers, "Specifications for Evaluation of Infrared Reference Spectra," *Anal. Chem.* **38**, 27A (1966).
(4) "Recommendations for Infrared Spectra of New Compounds," *Anal. Chem.* **40**, 2272 (1968).
(5) Kennard, O., J. C. Speakman, and J. D. H. Donnay, *Acta Crystallogr.* **22**, 445 (1967).
(6) Ibers, J. A., *Inorg. Chim. Acta* **3**, No. 3, Sept. 30, 1969 (9th prelim. page).
(7) McCullough, J. P., E. F. Westrum, Jr., and W. H. Evans, *Science* **132**, 1658 (1960).
(8) Sokolov, V. A., V. P. Kolesov, and A. F. Vorob'ev, *Zh. Fiz. Khim.* **39**, 1298 (1965).
(9) Rollefson, G. K., *J. Amer. Chem. Soc.* **77**, No. 10, p. iii (1965).
(10) Hanley, H., M. Klein, P. E. Lilley, S. C. Sazena, J. V. Sengers, G. Thodos, and H. J. White, Jr., "Recommendations for Data Compilations and for the Reporting of Measurements of the Thermal Conductivity of Gases," *J. Heat Transfer*, (1969), to be published.
(11) ASTM Committee E-19, "Proposed Recommended Practice for Gas Chromatography Terms and Relationships," *J. Gas Chromatog.* **6**, 1 (1968).
(12) "Guide for Measures of Precision and Accuracy," *Anal. Chem.* **40**, 2271 (1968).
(13) McAdie, H. G., *Anal. Chem.* **39**, 543 (1967).
(14) Meggers, W. F., and C. E. Moore, Joint Commission for Spectroscopy, *J. Opt. Soc. Amer.* **43**, 422 (1953).
(15) Jenkins, F. A., Joint Commission for Spectroscopy, *J. Opt. Soc. Amer.* **43**, 425 (1953).
(16) "Spectrometry Nomenclature," *Anal. Chem.* **40**, 2271 (1968).

Systems Requirements for Primary Information Systems

Utilization of *The Journal of Organic Chemistry**

JOSEPH H. KUNEY
American Chemical Society, 1155 Sixteenth St., N.W., Washington, D. C. 20036

WILLIAM H. WEISGERBER
Omnisearch, 632 McLean Ave., Yonkers, N. Y. 10705

Received January 19, 1970

A selected sample of 281 readers of *The Journal of Organic Chemistry* has been interviewed personally to obtain data on their reading patterns of the November 1968 issue. Approximately 35% of the individual subscribers to JOC had read or looked through the journal within the first seven days of receipt. The average reader claims to have read part or all of 14 articles out of the 81 available. At least 75% of every one of the 81 articles was read, ranging from a low of 0.7% to a high of 10.2%. Structures or equations rated high as a "noted" segment of an article. In addition to data on amount of reading of the issue, respondents were asked about amount of time spent reading, other journals read, and journals subscribed to. Correlations have been developed between subject interest as stated by respondent and his actual reading pattern.

Studies of the scientist's use of information are based on the premise that if we know what the scientist does with existing means, we can design new and better systems to serve him.[1,2,3] But with some few exceptions,[4] such studies have failed to relate the data generated to the specific problems facing the designer of information systems.

In this study of the reading behavior of the subscribers to *The Journal of Organic Chemistry*, we explore the possibilities of using the data generated as a basis for the design and test of new systems of disseminating and communicating scientific information—in particular, to relate such data to the problems of providing users with units of scientific information more closely matched to their interests and job-contact patterns whether the medium of transmission be the printed page or a computer console.

The primary objectives of this study were:

* Presented in part in Symposium on Who Reads the Chemical Literature and For What Purposes, Division of Chemical Literature, ACS National Meeting, New York, N. Y., September 8, 1969.