Reports

Calorimetry Group Adopts Revised Resolution on Data Publication

In 1953 the eighth Calorimetry Conference adopted a resolution outlining minimum publication standards for the guidance of authors, editors, and referees of calorimetric papers. Because this resolution has helped improve the quality of such papers, the 14th conference (1959) authorized the preparation of a revised resolution on publication that would be more consistent with the expanded scope of the conference and the present state of calorimetric science. The revised and expanded resolution that follows, "Resolution on Publication of Calorimetric and Thermodynamic Data," was adopted by the 15th conference at Gatlinburg, Tenn., 7–10 September 1960.

Introduction

This resolution is addressed not only to the specialist in calorimetry and chemical thermodynamics but also to those who determine and publish thermodynamic data as a subordinate part of their research. We urge all who publish thermodynamic data, for whatever purpose determined, to consider the suggestions to follow so that maximum benefits from their work may be realized. We also recommend this resolution to journal editors and referees as a set of carefully considered criteria for judging the completeness and acceptability of papers reporting calorimetric data.

General Philosophy

The very nature of chemical thermodynamics imposes special burdens on the author of a paper reporting the results of calorimetric investigations. Because the body of thermodynamic data is highly interdependent, he must give enough information about his experiments to allow others to appraise the precision and accuracy of his results for proper consolidation with the existing body of data. Further, as accepted values of physical constants change or as new thermodynamic data for related systems become available, later investigators often can recalculate results based on good calorimetery, however old it may be. For these reasons, an author's first responsibility is to report his results in a form related as closely to experimentally observed quantities as is practical, with enough details of the experiments and auxiliary information to characterize the results completely. For the convenience of the reader, the author should interpret and correlate the primary data, as appropriate, and present derived data in a form easy to use. However, derived or secondary data *never* should be published at the cost of omitting the primary data on which it is based.

Necessary Auxiliary Information

Detailed auxiliary information is required to characterize the results of any definitive thermodynamic study. Applicable items listed in the following paragraphs always should be given either in full or by reference to accessible earlier publications containing full details.

Apparatus and procedures. A complete description of the apparatus and procedures, including details of the reaction container or calorimeter vessel, the controlled environment, and the temperature and time measuring systems; the method of calibration and the sensitivity of measuring instruments such as thermometers, bridges and potentiometers, timing devices, and flow meters; the method of determining the energy equivalent of or otherwise calibrating the system; the observational procedure; the method of data reduction; and the precision and accuracy of the results obtained, preferably established by using recognized reference substances such as the Calorimetry Conference samples of *n*-heptane, benzoic acid, and aluminum oxide for heat capacity or enthalpy measurements.

Materials. The source of and/or method of preparing all materials used, including calibration, reference, and auxiliary substances; experimental values for analyses and pertinent physical properties of materials, and criteria of purity; and method of storing samples and preparing them for calorimetric measurements, if important.

Auxiliary data. Atomic or molecular weights; fundamental physical constants; temperature scales; units of energy and relationship between units; and values of thermochemical or thermodynamic data taken from the literature, with sources. The absolute joule or the defined thermochemical calorie equal to 4.184 absolute joules exactly and the International Temperature Scale, with the definition 0° Celsius (International) = 273.15° Kelvin (International), are recommended.

Presentation of Results

It is not practical to give detailed recommendations for presenting the results of all kinds of thermochemical or thermodynamic investigations. However, the following paragraphs (*1*) give recommendations for some important kinds of thermodynamic studies and will serve as guides for others.

Thermochemical data. The following experimental data should be included if applicable: Energy equivalent of the calorimetric system; mass of sample and/or mass of product used in determining the amount of reaction; masses of auxiliary substances; corrected temperature increment; total observed energy change; ignition energy; chemical and physical specification of the initial and final states of the reaction; conversion to "standard" concentrations; corrections for side reactions; allowances for energy changes due to flow of gases, stirring, or other effects; allowances for energy from auxiliary substances; reduction to standard states, such as the "Washburn corrections"; temperature of experiments; and final experimental heat of reaction and uncertainty interval, with the chemical reaction to which the result applies. If possible, derived data such as enthalpy and Gibbs free energy of formation should be given for the convenience of the reader.

Thermal data. The following information is considered indispensable for delineating the temperature dependence of thermodynamic properties of nonreacting systems, ascertaining the influence of thermal history on measured properties, and evaluating the precision of the results: A table of experimental values of heat capacity or enthalpy increment; the actual temperature increments used in the measurements when important (e.g., in transition, premelting, or anomalous regions), either explicitly or implicitly by chronological presentation of data or by a general statement; indication of values adjusted for curvature or premelting;

Instructions for preparing reports. Begin the report with an abstract of from 45 to 55 words. The abstract should *not* repeat phrases employed in the title. It should work with the title to give the reader a summary of the results presented in the report proper.

Type manuscripts double-spaced and submit one ribbon copy and one carbon copy.

Limit the report proper to the equivalent of 1200 words. This space includes that occupied by illustrative material as well as by the references and notes.

Limit illustrative material to *one* 2-column figure (that is, a figure whose width equals two columns of text) or to *one* 2-column table or to *two* 1-column illustrations, which may consist of two figures or two tables or one of each.

For further details see "Suggestions to Contributors" [*Science* **125**, 16 (1957)].

values of the heat and temperature of essentially isothermal phase changes; and an estimate of the accuracy uncertainty of the results. These primary experimental data should be supplemented, but never supplanted, by a tabulation of smoothed values of thermodynamic properties at selected temperatures. Where applicable, such tabulations should include values of Gibbs free energy function, $(F-H°_0)/T$, enthalpy (heat content) function, $(H-H°_0/T$, entropy, S, heat capacity, C_p (or C_{sata}), and enthalpy, $H-H°_0$, at 5° intervals from 0 to 50°K, 10° intervals from 50 to 300°K or slightly higher temperatures, and 50° to 100° intervals at higher temperatures, with appropriately smaller intervals in regions of thermal anomaly. Values at the two important reference temperatures, 273.15 and 298.15°K, and at the temperatures of phase changes should be included in the tabulations. Graphical or analytical representation of the results is sometimes worth while for the convenience of the reader, but such representations seldom are a satisfactory substitute for tabular presentation of accurate experimental results.

Calculated thermodynamic functions. As the usefulness of calorimetric data often is extended by giving calculated thermodynamic functions based on them, recommendations for presenting this kind of thermodynamic data are included here. The following information, with sources, is needed to characterize the results of statistical thermodynamic calculations: Details of the molecular model used, including bond distances and angles, specification of the exact conformation, moments of inertia or rotational constants, and symmetry number; complete vibrational assignment; parameters used for calculating contributions of internal rotation, anharmonicity, centrifugal distortion, etc.; citation, usually by reference, of formulas and special tabulations used; comparison with experimental thermodynamic data when available; and tables of thermodynamic functions at selected temperatures. The functions tabulated should include all of the following: Gibbs free energy function, $(F° -H°_0)/T$; enthalpy (heat content) function, $(H° -H°_0)/T$; entropy, $S°$; heat capacity, $C_p°$; and enthalpy, $(H° -H°_0)$. In addition, values of enthalpy of formation, $\Delta Hf°$, Gibbs free energy of formation, $\Delta Ff°$, and common logarithm of the equilibrium constant of formation, $\log_{10}Kf$, may be published if warranted. The values should be reported at temperatures so spaced that no serious loss of accuracy will result by interpolation with a formula equivalent to 5-point Lagrangian interpolation; for example, at 50° intervals to 300°K, 100° intervals to 1500°K, 200° intervals to 2500°K, and 500° intervals at higher temperatures. Values also should be tabulated at the reference temperatures, 273.15 and 298.15°K.

Nondefinitive data. This resolution is concerned primarily with the publication of precise and accurate data taken by definitive techniques, but rough measurements often are made for technical purposes and these data occasionally are submitted for publication. As such measurements are sometimes made on materials of undefined composition or by techniques substantially inferior to those accepted as definitive, they clearly do not merit space in scientific journals on the same basis as definitive studies, and the foregoing recommendations do not apply in full. The same is true of calculated thermodynamic functions that are based on unsubstantiated or estimated molecular data and that are not verified by comparison with experimental thermodynamic data. However, even rough data or calculated values *may* be better than empirical estimates and, so, have some value, but they are of doubtful significance as a basis for many theoretical deductions or for incorporation in critical tables of scientific data. Therefore, it is recommended that minimum journal space be allotted to such results and that the presentation clearly recognize their lack of reliability. The use of the American Documentation Institute supplement may be appropriate for the bulk of such data, with the location attested only by a brief note in a journal.

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Ad Hoc Committee on Publications, 15th Calorimetry Conference

Note

1. The use herein of symbols and terminology accepted generally by American scientists is not intended as a recommendation of the Calorimetry Conference. Appropriate international organizations are now developing a uniform system of symbols and terminology for thermodynamics. Calorimetrists are urged to follow the international system when it is officially adopted.

21 October 1960

Action of 1-Benzyl-2-methyl-5-methoxytryptamine on Monoamine Oxidase

In their report on monoamine oxidase, psychoenergizers, and tranquilizers, A. Feldstein, H. Hoagland, and H. Freeman [*Science* **130**, 500 (1959)] cast "some doubt on the hypothesis that Marsilid [iproniazid] exerts its central stimulatory action by virtue of its ability to inhibit monoamine oxidase." Their objection to this hypothesis stems from the assumption that 1-benzyl-2-methyl-5-methoxytryptamine (BAS), a tranquilizing agent, and iproniazid, a psychoenergizer, both block monoamine oxidase. The authors interpret their data by referring to the work of D. W. Woolley *et al.* (*1*), who observed an increase of urinary serotonin excretion in mice after the administration of BAS and who ascribed this phenomenon to monoamine oxidase inhibition. However, no data have as yet been published regarding the influence of BAS on this enzyme.

Since the authors' argument against the monoamine oxidase hypothesis has already been repeated elsewhere (*2*) it seemed necessary to test directly the effect of BAS on monoamine oxidase. Recently this was done in my laboratory (*3*) with various preparations—for example, beef liver mitochondria and human and mouse liver homogenates which were suspended in tris-buffer. According to our standard procedure (*4*), the inhibitory power of BAS turned out to be very low ($pI_{50} \geqq 3$). It seems, therefore, not very likely that BAS acts by way of monoamine oxidase, and the biological effects of this substance, as described by Feldstein *et al.*, may have to be explained differently.

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References and Notes

1. D. W. Woolley and P. M. Edelman, *Science* **127**, 281 (1958).
2. Editorial, *Brit. Med. J.* **1959**, **II**, 1238 (1959); L. Rees, *Nature* **186**, 114 (1960).
3. I am indebted to Dr. D. W. Woolley for a sample of BAS. Most of the experiments were carried out by Sama E. Sama.
4. E. A. Zeller, J. Barsky, E. R. Berman, M. S. Cherkas, J. R. Fouts, *J. Pharmacol. Exptl. Therap.* **124**, 282 (1958).

16 June 1960

We reported (*1*) the administration of 100 mg of DL-5-hydroxytryptophan (DL-5-HTP) to patients pretreated with 1-benzyl-2-methyl-5-methoxytryptamine (BAS). We found, unexpectedly, small amounts of 5-hydroxyindoleacetic acid (5-HIAA) determined quantitatively by the Udenfriend extraction procedure and semiquantitatively by two-dimensional paper chromatograms of the neat urine. We also found major spots corresponding in R_F value and Ehrlich color to 5-hydroxytryptophan (5-HTP), 5-HIAA, and serotonin. We interpreted the data as meaning that BAS was a monoamine oxidase inhibitor which blocked the formation of 5-HIAA and caused an accumulation of serotonin.

Recently we investigated the intravenous administration of 5 μc of DL-5-HTP-C^{14} to five untreated chronic-schizophrenic patients. The recovery of urinary 5-HIAA-C^{14} based on administered counts was 22.0 percent.