Specifications and Criteria for Biochemical Compounds

THIRD EDITION including the Biogenic Amine Supplement

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THIRD EDITION
Including the
Biogenic Amine Supplement

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Prepared by the
Committee on Specifications and Criteria
for Biochemical Compounds
Division of Chemistry and
Chemical Technology
National Research Council

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3rd Edition

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This report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

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Preface

This publication is the result of a program to improve the quality of chemicals available for biochemical research by establishing criteria, standards, or specifications useful for describing such chemicals, particularly with regard to purity. These pages represent an effort to satisfy a long-felt need of biochemists for more knowledge of the chemicals used in their investigations.

The program was initiated by Dr. Sam R. Hall* who, as a result of discussion with prominent biochemists, brought the matter to the attention of the Biochemistry Study Section of the National Institutes of Health at its meeting of January 1955. The Study Section recommended that a joint committee be established by the two largest organized groups of biochemists, the American Society of Biological Chemists and the Division of Biological Chemistry of the American Chemical Society. The governing bodies of these societies referred the problem to the then newly formed Committee on Biological Chemistry of the Division of Chemistry and Chemical Technology, National Academy of Sciences-National Research Council. Under the chairmanship of Prof. Herbert E. Carter, this Committee surveyed the need by submitting a questionnaire to the memberships of both societies. The response was 42 percent (considerably beyond normal expectations), and about 90 percent of the replies indicated a serious need for improvement in the quality and the standards of biochemicals.† This response, together with many additional comments and communications, was regarded by the Committee on Biological Chemistry as a mandate for action.

Much of the earlier work on the project was carried out by the Committee on Biological Chemistry. However, the need for a continuing examination of problems in this area has been recognized by the formation of a Committee on Specifications and Criteria for Biochemical Compounds, a standing committee of the Division of Chemistry and Chemical Technology of the National Academy of Sciences-National Research Council. This committee has been responsible for preparing the third edition of this work. Many individuals were involved, and they relied heavily on the work of the numerous persons who contributed to the preparation of the earlier editions. A cumulative list of all the members of the former Committee on Biological Chemistry and the earlier subcommittees is to be found in the second edition, published in 1967. Following this preface is a list of present members of the Committee on Specifications and Criteria for Biochemical Compounds and its subcommittees. It should be realized that many other individuals helped immeasurably with the task of preparing this volume, and the Committee expresses its gratitude to these unnamed persons.

The principle guiding the Committee and its subcommittees has been to select those criteria and specifications that permit adequate characterization of quality for each compound included. For the sake of uniformity, the following definitions have been adopted as guidelines: *Criteria* state what a compound or material is, or what it does, or both; criteria describe any or all of the following: (a) chemical properties, (b) physical prop-

^{*} Dr. Hall was at that time Executive Secretary of the Endocrinology Study Section of the National Institutes of Health. He played a leading role in the early development of this program and remained active in it until he left NIH in 1956 to join the staff of the American Cancer Society.

[†] Science, 123, 54 (1956).

erties, (c) some kind of activity; criteria describe the properties of the purest and most highly active specimen reported to date. *Specifications* are based on criteria; they give acceptable ranges for the selected criteria and procedures for determining that these requirements have been met. Specifications may also describe properties that the material shall not possess, as well as requirements for preserving, handling, packaging, dating, and labeling.

Fine biochemicals—unlike inorganic chemicals—are supplied by a comparatively small number of specialized manufacturers who are, however, widely dispersed on this continent, as well as in Europe, Asia, and South America. The preparations may involve not only a variety of procedures, but also starting materials of various degrees of purity. Some classes of compounds, such as the sugars and amino acids, were relatively well characterized before this program was initiated. For those compounds, the criteria and specifications represent accurate descriptions of existing high-grade commercial preparations. Many other substances, however, such as the enzymes and coenzymes, cannot be described so rigorously. The subcommittees felt that it would be more appropriate to describe such substances in terms of criteria by which the user could form his own judgment as to their purity.

The Committee believes that the major burden of evaluating the acceptability of biochemicals for any specific use or purpose belongs, in the long run, to the users themselves. Although the representations of suppliers may generally be relied upon, users should be acquainted with the best available and practicable guide for recognizing the degree of purity required, and it should be the user's responsibility to determine what, if any, further purification may be needed. Many of the compounds for which criteria and specifications are given in this book are labile, and precautions should be taken to ensure their stability. Normally, recommendations of the manufacturer should be followed when storing these materials.

This edition contains criteria and specifications for 521 compounds. The first edition consisted of two volumes of loose-leaf pages, covering 225 compounds, and the second was a hard-cover volume containing data on 392 compounds.

Although there has been a progressive increase in the size of successive editions, the coverage is, of course, by no means complete. Each of the subcommittees has additional compounds under consideration for future editions, and other subcommittees will probably be appointed to consider categories of biochemicals not yet included. It is considered that the criteria and specifications here selected for the individual compounds constitute the best information available to date. In the future,

improved techniques will undoubtedly reveal better criteria, and improvements in manufacturing practice will put on the market products having a degree of purity not now commercially feasible.

The problem of setting criteria and specifications for radioactively labeled biochemicals is one that has long plagued the Committee, for it was realized that this Pandora's Box should be opened with care. Nevertheless, with so many labeled compounds available commercially, a start in this direction had to be made. As a first step, some general comments concerning the use of these materials are included in this volume, in a section prepared by Dr. Horace S. Isbell. For the performance of this task, the Committee is extremely grateful to Dr. Isbell, who has acquired an extensive knowledge of the problem through his many years of experience in the synthesis and use of isotopically labeled materials.

In accordance with unit prefixes and abbreviations recommended by the International Bureau of Weights and Measures,* nm has been used for nanometre (formerely, $m\mu$ for millimicron) and μ m for micrometre (formerly, μ for micron). Where the name in common use for a compound differs from that in the Subject Index to *Chemical Abstracts*, the latter name is usually given also (parenthetically in boldface type) in the heading for a specification.

The Committee on Specifications and Criteria for Biochemical Compounds would greatly appreciate having any errors or omissions found in this publication brought to its attention. This request is earnestly directed to all purchasers and other interested persons. The Committee is also eager to receive criticisms and suggestions regarding either substantive text or publication format. As in many ventures with multiple authorship, there have been differences of opinion on selection of information and on the best manner to assemble and present the material. It is hoped that suggestions from the scientific public will result in improvement of future editions.

Another important aspect is evaluation by users of the adequacy of the data in actual situations. If some users find, for example, that the specifications and criteria are of limited value to them because of the manner of presentation or because certain additional information is not supplied, these facts will be of interest to the Committee, and communications will be welcome. In this connection, it should be pointed out that the biochemical characterizations were developed for general use in research. The criteria and specifications of the biochemical materials in this publication relate to purity standards and not to use of the materials for pur-

^{* &}quot;The International System of Units (s1)," National Bureau of Standards Special Publication 330 (January 1971).

poses other than biochemical research. Users with special requirements should discuss their needs directly with the manufacturers.

Certain commercial products and instruments are identified in this publication in order to specify the experimental procedure in sufficient detail. In no case does such identification imply recommendation or endorsement by the National Academy of Sciences—National Research Council, nor does it imply that the product or equipment so identified is necessarily the best available for the purpose.

Reports of errors, suggestions for revisions, and other comment on either substance or format may be addressed to:

Committee on Specifications and Criteria for Biochemical Compounds Division of Chemistry and Chemical Technology National Academy of Sciences-National Research

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Council

In conclusion, the Committee expresses appreciation for encouragement and support by the National Institutes of Health under Contract PH 43-64-44, Task Order No. 13, without which this project could not have been realized. The Committee owes a special debt of gratitude to Dr. R. Stuart Tipson, who edited the manuscript. Thanks are owing also to Dr. Waldo E. Cohn, Director of the NAS-NRC Office of Biochemical Nomenclature, for valuable advice regarding approved nomenclature.

At Sigma, we have always found this book to be invaluable. This edition, as well as previous editions, has been routinely used in our laboratories over the years as a guide to confirm the purity of many of our biochemicals. Although the data contained herein is from 1972, or before, most of it is as ageless as the molecules themselves.

We were disappointed to learn that the third edition was no longer in print and that a subsequent edition had not been planned. We have therefore reprinted this information in order to make it available once again to the biochemical community.

We appreciate the cooperation of the National Academy of Sciences in granting us exclusive permission to reprint this work and thereby perpetuate this reference book.

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Note: The section on Amino Acids and Related Compounds has been carried over without revision from the second edition (1967). The Subcommittee active in the preparation of that section consisted of Clarence P. Berg (Chairman), E. E. Howe, Alton Meister, Karl Pfister III, and Halbert C. White.

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Acetic Acid	L-1	125
Propionic Acid		125
Butyric Acid		125
Isobutyric Acid		125
Crotonic Acid		125
3-Hydroxybutyric Acid		125
Valeric Acid		125
Table 2 for Normal Saturated Short-Chain Fatty Acids C ₆ through		126
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Pelargonic Acid		126 126
Capric Acid		
Hendecanoic Acid		126
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Table 3 for Saturated Long-Chain Fatty Acids $\geq C_{14}$		g 100.7%
Myristic Acid		127
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Lipids and Related Compounds (continued)	Code Number	P
Pentadecanoic Acid	L-18	1
12-Methyltetradecanoic Acid	L-19	1
Palmitic Acid	L-20	1
Isopalmitic Acid	L-21	1
Margaric Acid	L-22	1
Anteisomargaric Acid	L-23	1
Stearic Acid	L-24	1
Isostearic Acid		1
Nonadecanoic Acid	L-26	1
Arachidic Acid	L-27	1
Phytanic Acid	L-28	1
Heneicosanoic Acid	L-29	1
Behenic Acid		1
Tricosanoic Acid	L-31	1
Lignoceric Acid		1
Cerotic Acid	L-33	1
Table 4 for Unsaturated Long-Chain Fatty Acids		
Myristoleic Acid	T 24	1
Palmitoleic Acid		1
Palmitelaidic Acid		1
Petroselinic Acid		1
Oleic Acid		1
Elaidic Acid		1
cis-Vaccenic Acid.		1
trans-Vaccenic Acid		1
Linoleic Acid		1
Linoelaidic Acid		1
Linolenic Acid		1
cis-5-Eicosenoic Acid		1
Eicosenoic Acid		1
Arachidonic Acid		1
Eicosapentaenoic Acid		1
Erucic Acid		1
Docosahexaenoic Acid		1
Nervonic Acid		1
	, , , , , , , , L-J1	
Table 5 for Normal Saturated Short-Chain Methyl Esters < C ₁₄		
Methyl Butyrate		1
Methyl Caproate		1
Methyl Enanthate		1
Methyl Caprylate		1
Methyl Pelargonate		1
Methyl Caprate		1
Methyl Hendecanoate		1
Methyl Laurate		1
Methyl Tridecanoate	L -60	1
Table 6 for Saturated Long-Chain Methyl Esters $\geq C_{14}$		
Methyl Myristate	L-61	1
Methyl Isomyristate		1
Methyl Pentadecanoate		1
Methyl 12-Methyltetradecanoate		1
Methyl Palmitate		1