McGraw-Hill HANDBOOKS

LANGE'S Handbook of CHEMISTRY

15 th Ed.

J. A. Dean

三氏化学手册

第15版

McGraw-Hill Book Co 浴界图と出版公司

LANGE'S HANDBOOK OF CHEMISTRY

John A. Dean

Professor Emeritus of Chemistry University of Tennessee, Knoxville

Fifteenth Edition

McGRAW-HILL, INC.

New York St. Louis San Francisco Auckland Bogotá Caracas Lisbon London Madrid Mexico Milan Montreal New Delhi Paris San Juan São Paulo Singapore Sydney Tokyo Toronto

ABOUT THE EDITOR

John A. Dean assumed the editorship of *Lange's Handbook of Chemistry* in 1968 with the Eleventh Edition. He is currently Professor Emeritus of Chemistry at the University of Tennessee at Knoxville. The author of nine major chemistry reference books used throughout the world, John Dean's research interests, reflected in over 105 research papers and scholarly publications, include instrumental methods of analysis, flame emission and atomic absorption spectroscopy, chromatographic and solvent extraction methods, and polarography. He received his B.S., M.S., and Ph.D. in Chemistry from the University of Michigan at Ann Arbor. In 1974, he was given the Charles H. Stone Award by the Carolina-Piedmont Section of the American Chemical Society. In 1991, he was awarded the Distinguished Service Award by the Society for Applied Spectroscopy; by the same organization he was awarded Honorary Membership in 1997.

书 名: Lange's Handbook of Chemistry, 15th ed.

作 者: J.A. Dean

中 译 名: 兰氏化学手册 第15版

出 版 者: 世界图书出版公司北京公司

印刷者:北京中西印刷厂

发 行: 世界图书出版公司北京公司 (北京朝内大街 137 号 100010)

开 本: 1/20 787×1245

印 张: 78

出版年代: 1999年10月

书 号: ISBN 7-5062-1477-6/O • 282

版权登记: 图字 01-1999-2723

定 价: 360.00 元

世界图书出版公司北京公司已获得 McGraw-Hill Book Co. Singapore 授权在中国大陆独家重印发行。

Copyright © 1999, 1992, 1985, 1979, 1973, 1967, 1961, 1956 by McGraw-Hill, Inc. All rights reserved.

Copyright renewed 1972 by Norbert Adolph Lange.

Copyright 1952, 1949,1946, 1944, 1941, 1939, 1937, 1934 by McGraw-Hill, Inc. All rights reserved. Except as permitted under the United States Copyright Act of 1976, no part of this publication may be reproduced or distributed in any form or by any means, or stored in a data base or retrieval system, without the prior written permission of the publisher.

ISBN 0-07-016384-7

Copyright © 1999 by The McGraw-Hill Companies, Inc. All rights reserved. Jointly Publishes by Beijing World Publishing Corporation/McGraw-Hill. This edition may be sold in the People's Republic of China only. This book cannot be re-exported and is not for sale outside the People's Republic of China.

IE ISBN 0-07-116202-X

Information contained in this work has been obtained by McGraw-Hill, Inc., from sources believed to be reliable. However, neither McGraw-Hill nor its authors guarantee the accuracy or completeness of any information published herein and neither McGraw-Hill nor its authors shall be responsible for any errors, omissions, or damages arising out of use of this information. This work is published with the understanding that McGraw-Hill and its authors are supplying information but are not attempting to render engineering or other professional services. If such services are required, the assistance of an appropriate professional should be sought.

PREFACE TO FIFTEENTH EDITION

This new edition, the fifth under the aegis of the present editor, remains the one-volume source of factual information for chemists, both professionals and students—the first place in which to "look it up" on the spot. The aim is to provide sufficient data to satisfy all one's general needs without recourse to other reference sources. A user will find this volume of value as a time-saver because of the many tables of numerical data which have been especially compiled.

Descriptive properties for a basic group of approximately 4300 organic compounds are compiled in Section 1, an increase of 300 entries. All entries are listed alphabetically according to the senior prefix of the name. The data for each organic compound include (where available) name, structural formula, formula weight, Beilstein reference (or if unavailable, the entry to the *Merck Index*, 12th ed.), density, refractive index, melting point, boiling point, flash point, and solubility (citing numerical values if known) in water and various common organic solvents. Structural formulas either too complex or too ambiguous to be rendered as line formulas are grouped at the bottom of each facing double page on which the entries appear. Alternative names, as well as trivial names of long-standing usage, are listed in their respective alphabetical order at the bottom of each double page in the regular alphabetical sequence. Another feature that assists the user in locating a desired entry is the empirical formula index.

Section 2 on General Information, Conversion Tables, and Mathematics has had the table on general conversion factors thoroughly reworked. Similarly the material on Statistics in Chemical Analysis has had its contents more than doubled.

Descriptive properties for a basic group of inorganic compounds are compiled in Section 3, which has undergone a small increase in the number of entries. Many entries under the column "Solubility" supply the reader with precise quantities dissolved in a stated solvent and at a given temperature.

Several portions of Section 4, Properties of Atoms, Radicals, and Bonds, have been significantly enlarged. For example, the entries under "Ionization Energy of Molecular and Radical Species" now number 740 and have an additional column with the enthalpy of formation of the ions. Likewise, the table on "Electron Affinities of the Elements, Molecules, and Radicals" now contains about 225 entries. The Table of Nuclides has material on additional radionuclides, their radiations, and the neutron capture cross sections.

Revised material for Section 5 includes the material on surface tension, viscosity, dielectric constant, and dipole moment for organic compounds. In order to include more data at several temperatures, the material has been divided into two separate tables. Material on surface tension and viscosity constitute the first table with 715 entries; included is the temperature range of the liquid phase. Material on dielectric constant and dipole moment constitute another table of 1220 entries. The additional data at two or more temperatures permit interpolation for intermediate temperatures and also permit limited extrapolation of the data. The Properties of Combustible Mixtures in Air has been revised and expanded to include over 450 compounds. Flash points are to be found in Section 1. Completely revised are the tables on Thermal Conductivity for gases, liquids, and solids. Van der Waals' constants for gases has been brought up to date and expanded to over 500 substances.

Section 6, which includes Enthalpies and Gibbs Energies of Formation, Entropies, and Heat Capacities of Organic and Inorganic Compounds, and Heats of Melting, Vaporization, and Sublimation and Specific Heat at Various Temperatures for organic and inorganic compounds, has expanded by 11 pages, but the major additions have involved data in columns where it previously was absent. More material has also been included for critical temperature, critical pressure, and critical volume.

The section on Spectroscopy has been retained but with some revisions and expansion. The section includes ultraviolet-visible spectroscopy, fluorescence, infrared and Raman spectroscopy, and X-ray spectrometry. Detection limits are listed for the elements when using flame emission, flame atomic absorption, electrothermal atomic absorption, argon induction coupled plasma, and flame atomic fluorescence. Nuclear magnetic resonance embraces tables for the nuclear properties of the elements, proton chemical shifts and coupling constants, and similar material for carbon-13, boron-11, nitrogen-15, fluorine-19, silicon-19, and phosphorus-31.

In Section 8, the material on solubility constants has been doubled to 550 entries. Sections on proton transfer reactions, including some at various temperatures, formation constants of metal complexes with organic and inorganic ligands, buffer solutions of all types, reference electrodes, indicators, and electrode potentials are retained with some revisions. The material on conductances has been revised and expanded, particularly in the table on limiting equivalent ionic conductances.

Everything in Sections 9 and 10 on physiochemical relationships, and on polymers, rubbers, fats, oils, and waxes, respectively, has been retained.

Section 11, Practical Laboratory Information, has undergone significant changes and expansion. Entries in the table on "Molecular Elevation of the Boiling Point" have been increased. McReynolds' constants for stationary phases in gas chromatography have been reorganized and expanded. The guide to ion-exchange resins and discussion is new and embraces all types of column packings and membrane materials. Gravimetric factors have been altered to reflect the changes in atomic weights for several elements. Newly added are tables listing elements precipitated by general analytical reagents, and giving equations for the redox determination of the elements with their equivalent weights. Discussion on the topics of precipitation and complexometric titrations include primary standards and indicators for each analytical technique. A new topic of masking and demasking agents includes discussion and tables of masking agents for various elements, for anions and neutral molecules, and common demasking agents. A table has been added listing the common amino acids with their pI and pK_a values and their 3-letter and 1-letter abbreviations. Lastly a 9-page table lists the threshold limit value (TLV) for gases and vapors.

As stated in earlier prefaces, every effort has been made to select the most useful and reliable information and to record it with accuracy. However, the editor's 50 years of

involvement with textbooks and handbooks bring a realization of the opportunities for gremlins to exert their inevitable mischief. It is hoped that users of this handbook will continue to offer suggestions of material that might be included in, or even excluded from, future editions and call attention to errors. These communications should be directed to the editor. The street address will change early in 1999, as will the telephone number. However, the e-mail address should remain as "pd105@aol.com."

Knoxville, TN

John A. Dean

PREFACE TO FOURTEENTH EDITION

Perhaps it would be simplest to begin by stating the ways in which this new edition, the fourth under the aegis of the present editor, has *not* been changed. It remains the one-volume source of factual information for chemists, both professionals and students—the first place in which to "look it up" on the spot. The aim is to provide sufficient data to satisfy all one's general needs without recourse to other reference sources. Even the worker with the facilities of a comprehensive library will find this volume of value as a time-saver because of the many tables of numerical data which have been especially compiled.

The changes, however, are both numerous and significant. First of all, there is a change in the organization of the subject matter. For example, material formerly contained in the section entitled Analytical Chemistry is now grouped by operational categories: spectroscopy; electrolytes, electromotive force, and chemical equilibrium; and practical laboratory information. Polymers, rubbers, fats, oils, and waxes constitute a large independent section.

Descriptive properties for a basic group of approximately 4000 organic compounds are compiled in Section 1. These follow a concise introduction to organic nomenclature, including the topic of stereochemistry. Nomenclature is consistent with the 1979 rules of the Commission on Nomenclature, International Union of Pure and Applied Chemistry (IUPAC). All entries are listed alphabetically according to the senior prefix of the name. The data for each organic compound include (where available) name, structural formula, formula weight, Beilstein reference, density, refractive index, melting point, boiling point, flash point, and solubility (citing numerical values if known) in water and various common organic solvents. Structural formulas either too complex or too ambiguous to be rendered as line formulas are grouped at the bottom of the page on which the entries appear. Alternative names, as well as trivial names of long-standing usage, are listed in their respective alphabetical order at the bottom of each page in the regular alphabetical sequence. Another feature that assists the user in locating a desired entry is the empirical formula index.

Section 2 combines the former separate section on Mathematics with the material involving General Information and Conversion Tables. The fundamental physical constants reflect values recommended in 1986. Physical and chemical symbols and definitions have undergone extensive revision and expansion. Presented in 14 categories, the entries follow recommendations published in 1988 by the IUPAC. The table of abbreviations and standard letter symbols provides, in a sense, an alphabetical index to the foregoing tables. The table of conversion factors has been modified in view of recent data and inclusion of SI units; cross-entries for "archaic" or unusual entries have been curtailed.

Descriptive properties for a basic group of approximately 1400 inorganic compounds are compiled in Section 3. These follow a concise, revised introduction to inorganic nomenclature that follows the recommendations of the IUPAC published in 1990. In this section are given the exact atomic (or formula) weight of the elements accompanied, when available, by the uncertainty in the final figure given in parentheses.

In Section 4 the data on bond lengths and strengths have been vastly increased so as to include not only the atomic and effective ionic radii of elements and the covalent radii for atoms, but also the bond lengths between carbon and other elements and between elements other than carbon. All lengths are given in picometers (SI unit). Effective ionic radii are tabulated as a function of ion charge and coordination number. Bond dissociation energies are given in kilojoules per mole with the uncertainty of the final figure(s) given in parentheses when known. New tables include bond dipole moments, group dipole moments, work functions of the elements, and relative abundances of the naturally occurring elements. The table of nuclides has been shortened and includes only the more commonly encountered nuclides; tabulations list half-life, natural abundance, cross-section to thermal neutrons, and radiation emitted upon disintegration. Entries have been updated.

Revised material in Section 5 includes an extensive tabulation of binary and ternary azeotropes comprising approximately 850 entries. Over 975 compounds have values listed for viscosity, dielectric constant, dipole moment, and surface tension. Whenever possible, data for viscosity and dielectric constant are provided at two temperatures to permit interpolation for intermediate temperatures and also to permit limited extrapolation of the data. The dipole moments are often listed for different physical states. Values for surface tension can be calculated over a range of temperatures from two constants that can be fitted into a linear equation. Also extensively revised and expanded are the properties of combustible mixtures in air. A table of triple points has been added.

The tables in Section 6 contain values of the enthalpy and Gibbs energy of formation, entropy, and heat capacity at five temperatures for approximately 2000 organic compounds and 1500 inorganic compounds, many in more than one physical state. Separate tabulations have enthalpies of melting, vaporization, transition, and sublimation for organic and inorganic compounds. All values are given in SI units (joule) and have been extracted from the latest sources such as JANAF Thermochemical Tables, 3d ed. (1986); Thermochemical Data of Organic Compounds, 2d ed. (1986); and Enthalpies of Vaporization of Organic Compounds, published under the auspices of the IUPAC (1985). Also updated is the material on critical properties of elements and compounds.

The section on Spectroscopy has been expanded to include ultraviolet-visible spectroscopy, fluorescence, Raman spectroscopy, and mass spectroscopy. Retained sections have been thoroughly revised: in particular, the tables on electronic emission and atomic absorption spectroscopy, nuclear magnetic resonance, and infrared spectroscopy. Detection limits are listed for the elements when using flame emission, flame atomic absorption, electrothermal atomic absorption, argon ICP, and flame atomic fluorescence. Nuclear magnetic resonance embraces tables for the nuclear properties of the elements, proton chemical shifts and coupling constants, and similar material for carbon-13, boron-11, nitrogen-15, fluorine-19, silicon-29, and phosphorus-31.

Section 8 now combines all the material on electrolytes, electromotive force, and chemical equilibrium, some of which had formerly been included in the old "Analytical Chemistry" section of earlier editions. Material on the half-wave potentials of inorganic and organic materials has been thoroughly revised. The tabulation of the potentials of the elements and their compounds reflects recent IUPAC (1985) recommendations.

An extensive new Section 10 is devoted to polymers, rubbers, fats, oils, and waxes. A discussion of polymers and rubbers is followed by the formulas and key properties of plastic materials. For each member and type of the plastic families there is a tabulation of their physical, electrical, mechanical, and thermal properties and characteristics. A similar treatment is accorded the various types of rubber materials. Chemical resistance and gas permeability constants are also given for rubbers and plastics. The section concludes with various constants of fats, oils, and waxes.

The practical laboratory information contained in Section 11 has been gathered from many of the previous sections of earlier editions. This material has been supplemented with new material under separation methods, gravimetric and volumetric analysis, and laboratory solutions. Significant new tables under separation methods include: properties of solvents for chromatography, solvents having the same refractive index and the same density, McReynolds' constants for stationary phases in gas chromatography, characteristics of selected supercritical fluids, and typical performances in HPLC for various operating conditions. Under gravimetric and volumetric analysis, gravimetric factors, equations and equivalents for volumetric analysis, and titrimetric factors have been retained

along with the formation constants of EDTA metal complexes. In this age of awareness of chemical dangers, tables have been added for some common reactive and incompatible chemicals, chemicals recommended for refrigerated storage, and chemicals which polymerize or decompose on extended storage at low temperature. Updated is the information about the U.S. Standard Sieve Series. Thermometry data have been revised to bring them into agreement with the new International Temperature Scale–1990, and data for type N thermocouples are included.

Every effort has been made to select the most useful and most reliable information and to record it with accuracy. However, the editor's many years of involvement with handbooks bring a realization of the opportunities for gremlins to exert their inevitable mischief. It is hoped that users of this handbook will offer suggestions of material that might be included in, or even excluded from, future editions and call attention to errors. These communications should be directed to the editor at his home address (or by telephone).

John A. Dean

PREFACE TO FIRST EDITION

This book is the result of a number of years' experience in the compiling and editing of data useful to chemists. In it an effort has been made to select material to meet the needs of chemists who cannot command the unlimited time available to the research specialist, or who lack the facilities of a large technical library which so often is not conveniently located at many manufacturing centers. If the information contained herein serves this purpose, the compiler will feel that he has accomplished a worthy task. Even the worker with the facilities of a comprehensive library may find this volume of value as a time-saver because of the many tables of numerical data which have been especially computed for this purpose.

Every effort has been made to select the most reliable information and to record it with accuracy. Many years of occupation with this type of work bring a realization of the opportunities for the occurrence of errors, and while every endeavor has been made to prevent them, yet it would be remarkable if the attempts towards this end had always been successful. In this connection it is desired to express appreciation to those who in the past have called attention to errors, and it will be appreciated if this be done again with the present compilation for the publishers have given their assurance that no expense will be spared in making the necessary changes in subsequent printings.

It has been aimed to produce a compilation complete within the limits set by the economy of available space. One difficulty always at hand to the compiler of such a book is that he must decide what data are to be excluded in order to keep the volume from becoming unwieldy because of its size. He can hardly be expected to have an expert's knowledge of all branches of the science nor the intuition necessary to decide in all cases which particular value to record, especially when many differing values are given in the literature for the same constant. If the expert in a particular field will judge the usefulness of this book by the data which it supplies to him from fields other than his specialty and not by the lack of highly specialized information in which only he and his co-workers are interested (and with which he is familiar and for which he would never have occasion to consult this compilation), then an estimate of its value to him will be apparent. However, if such specialists will call attention to missing data with which they are familiar and which they believe others less specialized will also need, then works of this type can be improved in succeeding editions.

Many of the gaps in this volume are caused by the lack of such information in the literature. It is hoped that to one of the most important classes of workers in chemistry, namely the teachers, the book will be of value not only as an aid in answering the most varied questions with which they are confronted by interested students, but also as an inspiration through what it suggests by the gaps and inconsistencies, challenging as they do the incentive to engage in the creative and experimental work necessary to supply the missing information.

While the principal value of the book is for the professional chemist or student of chemistry, it should also be of value to many people not especially educated as chemists. Workers in the natural sciences—physicists, mineralogists, biologists, pharmacists, engineers, patent attorneys, and librarians—are often called upon to solve problems dealing with the properties of chemical products or materials of construction. For such needs this compilation supplies helpful information and will serve not only as an economical substitute for the costly accumulation of a large library of monographs on specialized subjects, but also as a means of conserving the time required to search for

information so widely scattered throughout the literature. For this reason especial care has been taken in compiling a comprehensive index and in furnishing cross references with many of the tables.

It is hoped that this book will be of the same usefulness to the worker in science as is the dictionary to the worker in literature, and that its resting place will be on the desk rather than on the bookshelf.

Cleveland, Ohio May 2, 1934 N. A. Lange

ACKNOWLEDGMENTS

Grateful acknowledgment is hereby made of an indebtedness to those who have contributed to previous editions and whose compilations continue in use in this edition. In particular, acknowledgment is made of the contribution of L. P. Buseth, who prepared the conversion tables for the thirteenth edition and who prepared the table on the U.S. Standard Sieve Series.

CONTENTS

For the detailed contents of any section, consult the title page of that section. See also the alphabetical index in the back of this handbook.

Preface to Fifteenth Edition vii
Preface to Fourteenth Edition xi
Preface to First Edition xv
Acknowledgments xvii

Section	1.	Organic Compounds	1.1
Section	2.	General Information, Conversion Tables, and Mathematics	2.1
Section	3.	Inorganic Compounds	3.1
Section	4.	Properties of Atoms, Radicals, and Bonds	4.1
Section	5.	Physical Properties	5.1
Section	6.	Thermodynamic Properties	6.1
Section	7.	Spectroscopy	7.1
Section	8.	Electrolytes, Electromotive Force, and Chemical	
		Equilibrium	8.1
Section	9.	Physicochemical Relationships	9.1
Section	10.	Polymers, Rubbers, Fats, Oils, and Waxes	10.1
Section	11.	Practical Laboratory Information	11.1

Index follows Section 11

SECTION 1

ORGANIC COMPOUNDS

1.1 NOMENC	LATURE OF ORGANIC COMPOUNDS	1.1
1.1.1 Nonfund	ctional Compounds	1.1
Table 1.1	Names of Straight-Chain Alkanes	1.2
Table 1.2	Fused Polycyclic Hydrocarbons	1.8
Table 1.3	Specialist Nomenclature for Heterocyclic Systems	1.11
Table 1.4	Suffixes for Specialist Nomenclature of Heterocyclic Systems	1.12
Table 1.5	Trivial Names of Heterocyclic Systems Suitable for Use in Fusion	
	Names	1.13
Table 1.6	Trivial Names for Heterocyclic Systems That Are Not Recommended	
	for Use in Fusion Names	1.16
1.1.2 Function	nal Compounds	1.17
Table 1.7	Characteristic Groups for Substitutive Nomenclature	1.18
Table 1.8	Characteristic Groups Cited Only as Prefixes in Substitutive	
	Nomenclature	1.19
Table 1.9	Functional Class Names Used in Radicofunctional Nomenclature	1.22
1.1.3 Specific	Functional Groups	1.23
Table 1.10	Retained Trivial Names of Alcohols and Phenols with Structures	1.24
Table 1.11	Names of Some Carboxylic Acids	1.30
Table 1.12	Parent Structures of Phosphorus-Containing Compounds	1.36
1.1.4 Stereoc	hemistry	1.39
1.1.5 Chemica	al Abstracts Indexing System	1.49
Table 1.13	Names and Formulas of Organic Radicals	1.51
1.2 PHYSICAL	PROPERTIES OF PURE SUBSTANCES	1.58
Table 1.14	Empirical Formula Index of Organic Compounds	1.58
Table 1 15	Physical Constants of Organic Compounds	174

1.1 NOMENCLATURE OF ORGANIC COMPOUNDS

The following synopsis of rules for naming organic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see J. Rigaudy and S. P. Klesney, *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979. This publication contains the recommendations of the Commission on Nomenclature of Organic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).

1.1.1 Nonfunctional Compounds

1.1.1.1 Alkanes. The saturated open-chain (acyclic) hydrocarbons (C_nH_{2n+2}) have names ending in -ane. The first four members have the trivial names methane (CH_4) , ethane (CH_3CH_3) or C_2H_6 , propane (C_3H_8) , and butane (C_4H_{10}) . For the remainder of the alkanes, the first portion of the name

SECTION 1

ORGANIC COMPOUNDS

1.1 NOMENCI	ATURE OF ORGANIC COMPOUNDS	1.1
1.1.1 Nonfund	tional Compounds	1.1
Table 1.1	Names of Straight-Chain Alkanes	1.2
Table 1.2	Fused Polycyclic Hydrocarbons	1.8
Table 1.3	Specialist Nomenclature for Heterocyclic Systems	1.11
Table 1.4	Suffixes for Specialist Nomenclature of Heterocyclic Systems	1.12
Table 1.5	Trivial Names of Heterocyclic Systems Suitable for Use in Fusion	
	Names	1.13
Table 1.6	Trivial Names for Heterocyclic Systems That Are Not Recommended	
	for Use in Fusion Names	1.16
1.1.2 Function	al Compounds	1.17
Table 1.7	Characteristic Groups for Substitutive Nomenclature	1.18
Table 1.8	Characteristic Groups Cited Only as Prefixes in Substitutive	
	Nomenclature	1.19
Table 1.9	Functional Class Names Used in Radicofunctional Nomenclature	1.22
1.1.3 Specific	Functional Groups	1.23
Table 1.10	Retained Trivial Names of Alcohols and Phenols with Structures	1.24
Table 1.11	Names of Some Carboxylic Acids	1.30
Table 1.12	Parent Structures of Phosphorus-Containing Compounds	1.36
1.1.4 Stereoch	emistry	1.39
1.1.5 Chemica	I Abstracts Indexing System	1.49
Table 1.13	Names and Formulas of Organic Radicals	1.51
1.2 PHYSICAL	PROPERTIES OF PURE SUBSTANCES	1.58
Table 1.14	Empirical Formula Index of Organic Compounds	1.58
Table 1 15	Physical Constants of Organic Compounds	174

1.1 NOMENCLATURE OF ORGANIC COMPOUNDS

The following synopsis of rules for naming organic compounds and the examples given in explanation are not intended to cover all the possible cases. For a more comprehensive and detailed description, see J. Rigaudy and S. P. Klesney, *Nomenclature of Organic Chemistry*, Sections A, B, C, D, E, F, and H, Pergamon Press, Oxford, 1979. This publication contains the recommendations of the Commission on Nomenclature of Organic Chemistry and was prepared under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).

1.1.1 Nonfunctional Compounds

1.1.1.1 Alkanes. The saturated open-chain (acyclic) hydrocarbons (C_nH_{2n+2}) have names ending in -ane. The first four members have the trivial names methane (CH_4) , ethane (CH_3CH_3) or C_2H_6 , propane (C_3H_8) , and butane (C_4H_{10}) . For the remainder of the alkanes, the first portion of the name

1.2 SECTION 1

is derived from the Greek prefix (see Table 2.4) that cites the number of carbons in the alkane followed by -ane with elision of the terminal -a from the prefix, as shown in Table 1.1.

TABLE 1.1	Names	of Straight-Chain Alka	ines
-----------	-------	------------------------	------

n*	Name	n*	Name	n*	Name	n*	Name
1	Methane	11	Undecane‡	21	Henicosane	60	Hexacontane
2	Ethane	12	Dodecane	22	Docosane	70	Heptacontane
3	Propane	13	Tridecane	23	Tricosane	80	Octacontane
4	Butane	14	Tetradecane			90	Nonacontane
5	Pentane	15	Pentadecane	30	Triacontane	100	Hectane
6	Hexane	16	Hexadecane	31	Hentriacontane	110	Decahectane
7	Heptane	17	Heptadecane	32	Dotriacontane	120	Icosahectane
8	Octane	18	Octadecane			121	Henicosahectane
9	Nonane†	19	Nonadecane	40	Tetracontane		
10	Decane	20	Icosane§	50	Pentacontane		

^{*} n = total number of carbon atoms.

For branching compounds, the parent structure is the longest continuous chain present in the compound. Consider the compound to have been derived from this structure by replacement of hydrogen by various alkyl groups. Arabic number prefixes indicate the carbon to which the alkyl group is attached. Start numbering at whichever end of the parent structure that results in the lowest-numbered locants. The arabic prefixes are listed in numerical sequence, separated from each other by commas and from the remainder of the name by a hyphen.

If the same alkyl group occurs more than once as a side chain, this is indicated by the prefixes di-, tri-, tetra-, etc. Side chains are cited in alphabetical order (before insertion of any multiplying prefix). The name of a complex radical (side chain) is considered to begin with the first letter of its complete name. Where names of complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest-numbered locant at the first cited point of difference in the radical. If two or more side chains are in equivalent positions, the one to be assigned the lowest-numbered locant is that cited first in the name. The complete expression for the side chain may be enclosed in parentheses for clarity or the carbon atoms in side chains may be indicated by primed locants.

If hydrocarbon chains of equal length are competing for selection as the parent, the choice goes in descending order to (1) the chain that has the greatest number of side chains, (2) the chain whose side chains have the lowest-numbered locants, (3) the chain having the greatest number-of carbon atoms in the smaller side chains, or (4) the chain having the least-branched side chains.

These trivial names may be used for the unsubstituted hydrocarbon only:

Univalent radicals derived from saturated unbranched alkanes by removal of hydrogen from a terminal carbon atom are named by adding -yl in place of -ane to the stem name. Thus the alkane

[†] Formerly called enneane.

[‡] Formerly called hendecane.

[§] Formerly called eicosane.