

JOHN A. DEAN

LANGE'S HANDBOOK  
OF CHEMISTRY



FOURTEENTH EDITION

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**LANGE'S  
HANDBOOK  
OF  
CHEMISTRY**

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## ABOUT THE EDITOR

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John A. Dean assumed 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 100 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. In 1991, he was awarded the Distinguished Service Award by the Society for Applied Spectroscopy.

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# PREFACE TO FOURTEENTH EDITION

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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 spectrometry. 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).

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*John A. Dean*

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# PREFACE TO THIRTEENTH EDITION

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In this edition, the third under the aegis of the present editor, the large section devoted to the general description of 7600 organic compounds has been thoroughly revised. Nomenclature is now consistent with the 1979 rules of the Commission on Nomenclature, International Union of Pure and Applied Chemistry. A synopsis of the extensive nomenclature rules precedes the tabulation. All entries are listed alphabetically according to the senior prefix of the name rather than by indexing according to the Chemical Abstracts system. With the latter system there may be a bewildering array of subordinate entries listed under a key index name. The data for each organic compound include: name, structural formula, formula weight, Beilstein reference, density, refractive index, melting point, boiling point, flash point (introduced for the first time), and solubility in water and various organic solvents. Structural formulas are drawn for compounds either too complex or ambiguous to render by line formulas; these are grouped at the bottom of the same page on which the entry appears rather than being gathered together in a remote and separate listing. Many compounds will possess more than one approved name. These alternative names, as well as trivial names in long-standing usage, are listed in their respective alphabetical order at the bottom of each main page in the regular alphabetical sequence. Another aid to assist the user in locating a desired entry is the empirical formula index.

Expanded coverage is given to the areas of:

$pK_a$  values of organic acids

Temperature dependence of selected values of  $pK_a$  and  $pK_{sp}$  in water

Properties of combustible mixtures; in particular, the autoignition temperature and the flammable limits in percent by volume, upper and lower limits

The section on thermodynamic properties has been revised to reflect the latest recommended values for heats of formation and Gibbs energies of formation, entropies, and heat capacities for the members of the alkali family and the compounds of uranium, protactinium, thorium, and actinium. These data, plus heats of melting, vaporization, and sublimation, are gathered into two sets of two tables each, one for 2400 inorganic compounds and the other for 1500 organic compounds. The editor feels that related properties are thus more readily available to the user than if they were scattered over several separate tabulations.

Offered for the first time are carbon-13 NMR data involving chemical shifts and spin-spin coupling constants. This addition recognizes the increased role played by carbon-13 NMR in the elucidation of chemical structures.

In response to user requests, gravimetric conversion factors, equations and equivalents for volumetric analyses, standard volumetric solutions, and volumetric factors have been restored and updated in this edition.

The mathematical section has been restructured to exclude the tables for logarithms and trigonometric functions, data now easily obtained with the ubiquitous hand calculator.



This Handbook still remains the only one-volume source for extensive entries involving solubility products, the estimation of vapor pressure at various temperatures for inorganic and organic compounds—Antoine equation data, formation constants of metal complexes both inorganic and organic, equivalent conductance, critical volumes among the other critical data of temperature and pressure, and Hammett and Taft substituent constants.

Grateful acknowledgment is extended to Mr. L. P. Buseth (Norway) who consented to revise the table of conversion factors in Section 2.

It is hoped that users of this edition will continue to offer friendly criticism and suggestions and call attention to errors. These communications should be directed to the editor at his home address.

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# PREFACE TO FIRST EDITION

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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*

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# ACKNOWLEDGMENTS

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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 and offered revisions for this edition and who prepared the table on the U.S. Standard Sieve Series.

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# SECTION 1

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## ORGANIC COMPOUNDS

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### 1.1 NOMENCLATURE OF ORGANIC COMPOUNDS

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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 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 Alkanes

$n^*$	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	Hectaane
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.

† Formerly called enneane.

‡ Formerly called hendecane.

§ Formerly called eicosane.

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:

Isobutane  $(\text{CH}_3)_2\text{CHCH}_3$

Neopentane  $(\text{CH}_3)_4\text{C}$

Isopentane  $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$

Isohexane  $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3$

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

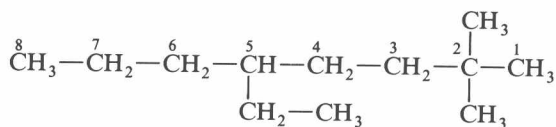
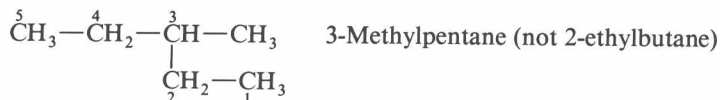


the alkane *ethane* becomes the radical *ethyl*. These exceptions are permitted for unsubstituted radicals only:

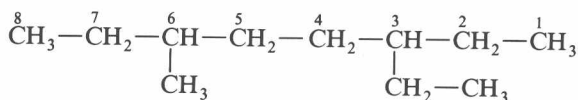
Isopropyl	$(\text{CH}_3)_2\text{CH}-$	Isopentyl	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2-$
Isobutyl	$(\text{CH}_3)_2\text{CHCH}_2-$	Neopentyl	$(\text{CH}_3)_3\text{CCH}_2-$
<i>sec</i> -Butyl	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-$	<i>tert</i> -Pentyl	$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2-$
<i>tert</i> -Butyl	$(\text{CH}_3)_3\text{C}-$	Isohexyl	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_2-$

Note the usage of the prefixes *iso*-, *neo*-, *sec*-, and *tert*-, and note when italics are employed. Italicized prefixes are never involved in alphabetization, except among themselves; thus *sec*-butyl would precede isobutyl, isohexyl would precede isopropyl, and *sec*-butyl would precede *tert*-butyl.

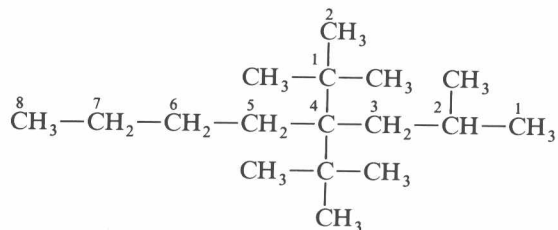
Examples of alkane nomenclature are



5-Ethyl-2,2-dimethyloctane (note cited order)



3-Ethyl-6-methyloctane (note locants reversed)



4,4-Bis(1,1-dimethylethyl)-2-methyloctane

4,4-Bis-1',1'-dimethylethyl-2-methyloctane

4,4-Bis(*tert*-butyl)-2-methyloctane

Bivalent radicals derived from saturated unbranched alkanes by removal of two hydrogen atoms are named as follows: (1) If both free bonds are on the same carbon atom, the ending -ane of the hydrocarbon is replaced with -ylidene. However, for the first member of the alkanes it is methylene rather than methyldiene. Isopropylidene, *sec*-butylidene, and neopentylidene