CRC

HANDBOOK *of* DATA *on* ORGANIC COMPOUNDS

2nd Edition

Volume X
1990 Update

Jeanette G. Grasselli

CRC PRESS

Handbook of Data on Organic Compounds

2nd Edition

Volume X
1990 Update

Editor

Jeanette G. Grasselli

CRC Press
Boca Raton Ann Arbor Boston

Library of Congress Cataloging-in-Publication Data
(Revised for volume)

Handbook of data on organic compounds.

Rev. ed. of: CRC handbook of data on organic compounds. c1985.
Includes indexes.
1. Organic compounds—Handbooks, manuals, etc.
I. Grasselli, Jeannette G. III. CRC Handbook of data on organic compounds.
QD257.7.H36 1991 547 90-24255
ISBN 0-8493-0420-2 (set)
ISBN 0-8493-0442-3

Direct all inquiries to CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, Florida 33431.

International Standard Book Number 0-8493-0442-3 (1990 update)

Library of Congress Card Number 90-24255

Printed in the United States

PREFACE TO VOLUME X: 1990 UPDATE

The *1990 Update* to the *Handbook of Data on Organic Compounds*, 2nd edition (HODOC II) continues in the style established for the basic, second edition volumes. All of the data for each compound appear in one location under the HODOC number for that compound. Chemical Abstracts Service Registry numbers have been provided for every compound.

For 986 compounds which previously appeared in HODOC II, additional data are presented in the *1990 Update* under the HODOC numbers previously assigned to the compounds. The new data for these compounds have been merged with the previously presented data to form a complete, unified body of data for the compound. In most cases, the additional data consist of spectral peaks.

In addition to the 986 compounds described above, data are presented for 1650 compounds new to HODOC II. These compounds have been assigned HODOC numbers, and the corresponding data are presented in the manner established by HODOC II.

The extensive set of indexes established for HODOC II continues in the *1990 Update*. Indexes within this volume are for those compounds and data appearing in the update. Utilizing the indexes, unknown compounds can be identified from characteristic physical constants or from spectral data.

Comments from users of HODOC II and the *1990 Update* are encouraged.

THE EDITOR

Jeanette G. Grasselli is a Distinguished Visiting Professor at Ohio University. She was formerly Director of Research and Analytical Sciences at the Research and Development Department of BP America, Cleveland, Ohio. Dr. Grasselli obtained her B.S. degree in chemistry at Ohio University, her M.S. at Case Western Reserve University, and has received D.Sc. (Hon.) degrees from Ohio University (1978) and Clarkson University (1986). She has 1 patent, 80 publications, and is co-editor of 8 books in the field of molecular spectroscopy. In 1970 she served as the National President of the Society for Applied Spectroscopy. She was active in organizing FACSS (The Federation of Analytical Chemistry and Spectroscopy Societies) and has been Chairman and Secretary of its Governing Board. She is on the Visiting Committee for the National Institute of Science and Technology (NBS), and serves on the Energy Research Advisory Board of the Department of Energy and the Chemical Sciences and Technology Board of the National Research Council. Dr. Grasselli is a Member of the U.S. National Committee for the International Union of Pure and Applied Chemistry (IUPAC), and is Secretary of the Spectroscopy Commission. She has received numerous awards and has been recognized for her many achievements in science, including the Anachem Award from the Detroit Association of Analytical Chemists, the Williams-Wright Award from the Coblentz Society, and the Garvan Medal of the American Chemical Society.

PREFACE

Chemists and engineers today have a greater need than ever before for easily accessible reference data. It is well recognized that the total number of organic compounds is growing rapidly, and physical data or information about them is often widely scattered throughout the literature. The second edition of the *CRC Handbook of Data on Organic Compounds* (HODOC II) is a reference source for physical and spectral data on the 26,000 most common organic compounds. This book incorporates not only a substantial revision of the first edition, but also now includes spectral data and/or references for many compounds. It therefore provides a comprehensive and unique database for identifying unknown compounds. It was our intent to provide a convenient, easy-to-use format on a reliable and important body of data for the industrial, academic, or government scientist.

All of the data for each compound in HODOC II appear in one location. The compounds are presented in alphabetical order by Chemical Abstracts Service (CAS) Chemical Index name. The IUPAC name, all common synonyms, the CAS number and the Beilstein number are given along with a HODOC II number for working with the various indexes. The Chemical Abstracts Service guide to naming chemical substances is reproduced in Volume I. This guide also includes molecular skeletons, stereochemistry, and chemical structural diagrams from CA index names. The molecular formula, molecular weight (calculated from the 1985 International Atomic Weights of the elements), line formula, and, in some cases, structure are given. The most recent physical property data available are listed and include the boiling point, melting point, density, refractive index, specific rotation, solubility, color, and crystalline form.

We have tried to present spectral information of uniformly high quality in a useful format. Our goal was to be concise and display the spectral information along with the other physical constants and information on each compound in the database. Careful coding criteria were established, the most reliable spectral reference catalogs were utilized, and a very sincere effort was made to evaluate the data as they were coded. It is worth noting, however, that the spectral data were coded with emphasis on selecting values characteristic of compound structure, not necessarily striving for a complete representation of the original spectrum.

A critical and truly unique feature of HODOC II is the extensive set of indexes which have been generated from the database. For example, there are 100,000 synonyms in the Synonym Index or an average of 4 synonyms per entry. There are also indexes for molecular formula, molecular weight, melting and boiling points, and 15 spectral indexes. The spectral indexes are for infrared, Raman, ultraviolet, H NMR, C NMR, and mass spectra, and these contain numerical indexes of source curves and special spectral data indexes subdivided by spectral region, chemical class, or band intensities (UV). Therefore, HODOC II can be used to obtain information, including spectral data, on approximately 26,000 compounds, or conversely, to identify an unknown from some characteristic physical constant or from spectral data.

Successful utilization of HODOC II depends upon recognition of the basic philosophy inherent in its organization and content. It is widely accepted that spectral data are of immense value in solving analytical problems, or in determining identity or structure of unknown materials. The enhanced status of spectroscopic methods should not contribute to a disregard for the importance of other physical constants of a substance. Certainly the most rapid and unambiguous identification of an unknown is often achieved by using several different physical properties. Toward this aim, this work provides a basic reference collection of physical constants and spectral data on organic compounds to facilitate such identifications. We well recognize that with the massive amount of data handled to assemble this book, errors or omissions are likely to be found. Corrections, criticism, and suggestions for improvement from users will be very welcome. It should be noted that HODOC II is a computer generated compendium. Therefore, some anomalies in generally accepted conventions for hyphenation of words, alphabetical sorting, etc. exist.

We intend to keep this extraordinary database current by publishing annual supplements. These will add new compounds, new data, and/or updated information on compounds listed in HODOC II. The supplements and this second edition of HODOC II will be available in computer-readable format as well as in bound volumes.

Many people have been involved in the preparation of HODOC II. We gratefully acknowledge the significant contribution of Chemical Abstract Services in providing Chemical Abstract numbers and names, and for verifying compound structures. Special recognition should be given to Jim Brody, Tom York, David Westbrook, Barbara Caras, Sandy Pearlman, Glenna Orsbin, and Robert Pitman of CRC Press, Inc., who had the overall responsibility for organizing the volumes of data and publishing the book. They did a superb job.

Jeanette G. Grasselli
Robert C. Weast

Handbook of Data on Organic Compounds, 2nd edition

Contents — Volumes I to IX

Introduction

EXPLANATIONS TO THE DATABASE

PHYSICAL PROPERTIES

HODOC Number

Abbreviation: HODOC No

HODOC is an acronym for *Handbook of Data on Organic Compounds*. The HODOC number is a numeric designation starting with 00001. The 00001 indicates the compound is the first compound in HODOC II, etc.

CAS Number

Abbreviation: CAS No

Data from the Chemical Abstracts Service (CAS) Registry System have been loaded into one file containing more than 7 million substances and more than 10 million names. The size of the file increases every week with routine updates. The original file contained CAS Registry Numbers only for compounds in the literature after 1965. Newly cited chemical compounds and substances from the current Pre-1965 Registration Project result in the addition of 10,000 to 15,000 substances to the CAS Registry File per week. Each unique chemical substance in the CAS Registry File has a unique Registry Number. CAS Registry Numbers of all compounds in HODOC II have been verified against CAS Registry Numbers in the CAS Registry File. Users will note that the CAS Registry Number always has from 2 to 6 digits to the left of the first dash, 2 numbers between the first and second dash, and only one number to the right of the second dash. Thus, a number might be 42-26-1 or 93673-25-0, but never 45-321-1 or 45-32-11.

Beilstein Number

Abbreviation: Beilstein No

All references are from the fourth edition of Beilstein's *Handbuch der Organische Chemie*. Nearly all of the references were checked by Beilstein personnel. Use of Beilstein is not difficult, but sometimes requires reading the instructions on its use. For example: 3^4,250 indicates the compound is listed on page 250 of the fourth supplement to Volume 3. Beilstein continues to be expanded. The fifth edition is in preparation and is being published in English.

Additional informational material on Beilstein is available upon request free of charge from:

Springer-Verlag KG
Heidelberger Platz 3
D-1000 Berlin 33

Springer-Verlag New York, Inc.
175 Fifth Avenue
New York, NY 10010

Name

The compound name listed for the compound is the name approved by the Chemical Abstracts Service as of late 1988. It is that name one would obtain first if one were to enter the Chemical Abstracts Service computerized databank via the CAS Registry Number. The Chemical Abstracts Service guide to naming chemical substances is reproduced in Volume I. This guide also includes molecular skeletons, stereochemistry, and chemical structural diagrams from CA index names.

Synonyms

The most common synonym for each compound is listed in the database. In addition, up to 100 synonyms known to the compilers and editors are included in the Synonym Index. All synonyms are listed in alphabetical order. For example, there are nine synonyms listed in the Synonym Index for the compound benzenamine, *N*-methyl (CAS Number 100-61-8). These are as follows: aniline, *N*-methyl; anilomethane; (methylamino)benzene; *N*-methylaniline; *N*-methylbenzenamine; methylphenylamine; *N*-methylamine; *N*-monomethylaniline; *N*-phenylmethylamine. Each synonym is followed by a HODOC II number which refers the searcher to the proper compound in the database where spectral information and physical properties for the compound can also be found.

Line Formula

Abbreviation: Line Form

The line formula presents the atoms in the way they are arranged in the molecule. Frequently, this is done by arranging the atoms in groups. For example, for ethanoic acid (CAS Number 64-19-7): CH_3COOH. Another example, *n*-octane (CAS Number 111-65-9), is written as $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$, whereas *iso*-octane or pentane, 2,2,4-trimethyl (CAS Number 540-84-1), is written as $CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$. Each of these last two named compounds has the molecular formula C_8H_{18}.

Structure

Structures, or as called by some persons, structural formulae, are presented when the systems are complicated or there is need to prevent ambiguity. Many structures are presented in the main database as part of the information on the compound. The Chemical Abstracts Service guide to naming chemical substances is reproduced in Volume I. This guide also includes molecular skeletons, stereochemistry, and chemical structural diagrams from CA index names.

Molecular Formula

Abbreviation: Mol Form

The molecular formula gives the types and numbers of atoms present in a molecule. Thus, the molecular formula for ethanoic acid (frequently called acetic acid) is

$C_2H_4O_2$. This is not the same as the *empirical formula* which lists the atoms in their simplest ratio. For ethanoic acid this would be CH_2O.

Molecular Weight
Abbreviation: M_r

Molecular weights for compounds were calculated using the 1985 International Atomic Weights of the elements. In HODOC II the *molecular weight* is treated the same as the *formula weight*. There are neither molecular weights nor formula weights listed for certain naturally occurring polymers, i.e., starch, whose degree of polymerization is unknown.

Boiling Point
Abbreviation: bp

The boiling point is given in °C at normal atmospheric pressure (760 mmHg, which equals 760 torr, or 101,325 pascals) unless indicated by a superscript to the numerical value for the boiling point. Thus, 58.4^{60} indicates the boiling point of 58.4°C was determined at a pressure of 60 mmHg which is equal to 60 torr. Pascals do not appear as a superscript for any data in this book. For some compounds there are two or more boiling points listed, with each boiliing point having been determined at a different pressure.

Melting Point
Abbreviation: mp

The melting point of a compound is listed in °C. Presence of the letters "d" or "dec" with the numerical value in the melting point column indicates the compound decomposes at the temperature listed. No distinction is made whether the decomposition occurs before the melting point is reached or if the compound decomposes during melting. Many compounds are salts or hydrates. Some of these lose an acid or water when heated. Such a reaction is indicated by -HCl (if the salt is a hydrochloride) or $-H_2O$ (if the compound is a hydrate) for the temperature at which the loss begins to occur.

Density
Abbreviation: *d*

Density is mass per unit volume. In SI units it is expressed as kg/m^3. However, most of the data in this book were obtained from publications wherein the density was expressed as g/cm^3. Unless indicated otherwise, density values are assumed to have been determined at laboratory room temperature. If the temperature was reported in the literature at which the determination was made, the density is followed by a superscript. Thus, 2.6372^{20} indicates the substance has a density of 2.6372 g/cm^3 at 20°C. If the density of the material is compared to the density of a reference material, frequently water, the number resulting from this ratio is called the *relative density*, formerly called *specific gravity*. *Relative density* is defined as the density of a substance relative to the density of some reference substance. For liquids or solids it is frequently the ratio of the density of the substance (usually at 20°C) to the density of water at its maximum density. The maximum density of water is at 3.98°C. However, most measurements are reported as being carried out at 4°C. The difference in density of water at 4°C and that at 3.98°C is less than usually necessary for relative density determinations. A *relative density* would be printed as $2.3480^{20/4}$. This number indicates the density of the substance was determined at 20°C and that this density was compared to that of water at 4°C. The ratio of the two densities is then reported as $2.3480^{20/4}$. It is understood that when the number 4 appears in the denominator of the superscript the reference material is water. If a substance other than water were used as the reference substance, that substance would be listed in the superscript.

Refractive Index
Abbreviation: *n*

The refractive index, which is also known as the refractive constant, is a function of the wavelength of light used to measure the refractive index. Thus the wavelength of light should be specified. The refractive index is usually determined using yellow light, the sodium D line, wavelength 589.3 nm. The numerical value for the refractive index should have a subscript indicating the wavelength of light used for the measurement. However, since the sodium D-line is most generally used, the subscript is either missing in some literature or appears as D. Thus 1.3446, $1.3446_{589.3}$, and 1.3446_D are identical. The temperature at which the refractive index is measured is frequently listed in the literature as a superscript to the numerical value. Thus, $1.5678^{23/D}$ is the numerical value of the refractive index of a compound when the measurement was made at 23°C and the sodium D-line was the light used. Refractive index is a ratio of the speed of electromagnetic radiation, nearly always light, in free space to the speed of the same radiation in another medium. Therefore, the number is dimensionless.

Specific Rotation
Abbreviation: α

Specific rotation, sometimes called optical rotation, is an optical property of a compound which is influenced by the wavelength of light used during the measurement, the length of the path through which the light passes, the particular solvent used to prepare a solution of the compound being studied, the concentration of the solution expressed in terms of the solute, and the temperature of the experiment. The path length of light through the experimental apparatus is usually 10 decimeters. This length is not always reported in the literature. Therefore, one needs to assume that if the length of the tube used in the experiment is not specified, the tube was 10 decime-

ters in length if the results are listed as specific rotation. Other controlled variables are nearly always listed. For example, $[\alpha]^{20/D} = +58°$ (c = 10% in C_2H_5OH) indicates that when 10 g of compound were dissolved in 100 g of C_2H_5OH and a beam of monochromatic light of wavelength 589.3 nm (the wavelength of the sodium D-line) passed through a tube of 10 decimeters in length containing the aforementioned solution at 20°C, the beam of light was rotated 58° to the right. If the light beam had been rotated to the left, a minus sign would have been in front of the numerical value of the rotation. Absence of square brackets around the α indicates the measurement was made without disolving the compound in a solvent, that is, the experiment was performed neat.

Color

The color and crystalline form of many compounds are listed in the database. The solvent from which the crystalline form is obtained is given in parentheses. Abbreviations for names of the colors and crystalline form are listed near the beginning of the database in the section *Abbreviations and Symbols*.

Solubility

Abbreviation: *s*

Quantitative data on solubilities rarely appear in the literature so a relative scale was established: 1 = insoluble, 2 = slightly soluble, 3 = soluble, 4 = very soluble, 5 = miscible, 6 = decomposes.

SPECTRAL DATA

Infrared, Raman, Ultraviolet, Nuclear Magnetic Resonance (^1H and ^{13}C), and Mass Spectral Data are given in the database. Either a reference to a spectral source curve or a coded representation of the spectrum is given for every compound. A complete listing of the reference collections used is given before the Numerical Index of Source Curves for every technique

Each curve was evaluated during the encoding procedure to guard against inclusion of impurity peaks or of anomalous absorptions. When more than one spectrum of the same compound was available, the one judged to be of highest quality was used. The coding of the spectral data was according to the following criteria.

Infrared

Abbreviation: IR

All absorption bands characteristic of the specific structure (i.e., the common group frequencies), regardless of intensity, were coded. In addition, at least one strong band in each micrometer or 100 cm^{-1} interval, from 3800 to 250 cm^{-1}, was coded. Spectra were coded in either micrometers or wavenumbers, depending on the format of the reference curve. Data in micrometers were converted by computer to wavenumbers for listing in the database and the Indexes (see Wavelength-Wavenumber Conversion Table). A micron symbol, μ, is shown before the spectrum reference number for every converted spectrum. Peak positions were read to ±0.1 μm or ±10 cm^{-1}. When a coder was unfamiliar with the structure and could not select the "most characteristic" bands, all medium to strong bands were coded.

Raman

The Raman spectra from the early API collection (#1-500) and those from the *Analytical Chemistry (AC)* reference article were obtained with a mercury arc source. Only the ten strongest bands in the spectra were coded. Spectra were only recorded from 1700 to 150 cm^{-1} in *AC* and this is indicated by an asterisk (*) before the first coded band. All other Raman spectra were generated using a laser source. These were coded over the range 4000 to 50 cm^{-1}. All recognized group frequencies and most significant bands were listed. In the Sadtler spectra only the parallel polarized curve was coded.

Ultraviolet

Abbreviation: UV

All bands, their molar absorption coefficients (in parentheses, when given), and the solvent used were coded. The wavelength range was from 170 to 600 nm and peaks were read to ±1 nm. When the spectrum showed vibrational fine structure, only the peak centers, characteristic of the electronic transitions, were read. If only a cut-off of absorption appeared, the notation b, for the peak below this wavelength, was used.

Nuclear Magnetic Resonance

Abbreviation: NMR

^1H — The proton chemical shifts, in ppm (δ), for specific protons or recognizable groups were coded to ±0.1 ppm over the range 0 to 15 ppm referenced to tetramethylsilane (TMS). When complex spectra due to second order effects or overlapping resonances were encountered, the range (indicated by connecting chemical shifts with a dash) was recorded. The solvent in which the spectrum was obtained was also coded, if known.

^{13}C — The carbon chemical shifts, in ppm (δ), for specific carbons or recognizable groups were coded to ±0.1 ppm over the range 0 to 200 ppm referenced to TMS. The solvent in which the spectrum was obtained was also coded, if known.

Mass Spectroscopy

Abbreviation: MS

The eight most abundant peaks, the parent peak (if not among the eight most abundant), and the relative intensities (in parentheses) were coded and are listed in order of decreasing intensity. If the parent peak was not observed

it is listed with an intensity of (0). All data are from magnetic sector spectrometers and were taken at normal (~70 ev) ionizing voltages.

m/e

The mass number or the m/e value of an ion is the quotient of the mass of that ion (given in atomic mass units) and its positive charge (number of electrons lost during ionization). One observes the value of m/e in HODOC II approximates closely to the molecular weight (M_r) listed for the compound. The molecular weight of a compound was calculated from the 1985 International Atomic Weights whereas the m/e was calculated from the atomic mass of the most abundant naturally occurring isotope of the element. Thus, when calculating the m/e ratio, one uses for hydrogen, 1.007825; for carbon, 12.0000; for nitrogen, 14.003074; for oxygen, 15.994915; for sulfur, 31.972070, for chlorine, 34.968852; etc. These atomic masses of the isotopes are presented in most books which contain data on the elements and their isotopes. Among these are the *CRC Handbook of Chemistry and Physics*, 69th edition, or *Table of Isotopes*, C. M. Lederer and V. S. Shirley, 7th edition, Wiley-Interscience. The m/e values listed in the database of HODOC II are for ions which have lost one electron.

Wavelength–Wavenumber Conversion Table

Wavelength, μm	Wavenumber, cm^{-1}									
	0	1	2	3	4	5	6	7	8	9
2.0	5000	4975	4950	4926	4902	4878	4854	4831	4808	4785
2.1	4762	4739	4717	4695	4673	4651	4630	4608	4587	4566
2.2	4545	4525	4505	4484	4464	4444	4425	4405	4386	4367
2.3	4348	4329	4310	4292	4274	4255	4237	4219	4202	4184
2.4	4167	4149	4132	4115	4098	4082	4065	4049	4032	4016
2.5	4000	3984	3968	3953	3937	3922	3906	3891	3876	3861
2.6	3846	3831	3817	3802	3788	3774	3759	3745	3731	3717
2.7	3704	3690	3676	3663	3650	3636	3623	3610	3597	3584
2.8	3571	3559	3546	3534	3521	3509	3497	3484	3472	3460
2.9	3448	3436	3425	3413	3401	3390	3378	3367	3356	3344
3.0	3333	3322	3311	3300	3289	3279	3268	3257	3247	3236
3.1	3226	3215	3205	3195	3185	3175	3165	3155	3145	3135
3.2	3125	3115	3106	3096	3086	3077	3067	3058	3049	3040
3.3	3030	3021	3012	3003	2994	2985	2976	2967	2959	2950
3.4	2941	2933	2924	2915	2907	2899	2890	2882	2874	2865
3.5	2857	2849	2841	2833	2825	2817	2809	2801	2793	2786
3.6	2778	2770	2762	2755	2747	2740	2732	2725	2717	2710
3.7	2703	2695	2688	2681	2674	2667	2660	2653	2646	2639
3.8	2632	2625	2618	2611	2604	2597	2591	2584	2577	2571
3.9	2564	2558	2551	2545	2538	2532	2525	2519	2513	2506
4.0	2500	2494	2488	2481	2475	2469	2463	2457	2451	2445
4.1	2439	2433	2427	2421	2415	2410	2404	2398	2392	2387
4.2	2381	2375	2370	2364	2358	2353	2347	2342	2336	2331
4.3	2326	2320	2315	2309	2304	2299	2294	2288	2283	2278
4.4	2273	2268	2262	2257	2252	2247	2242	2237	2232	2227
4.5	2222	2217	2212	2208	2203	2198	2193	2188	2183	2179
4.6	2174	2169	2165	2160	2155	2151	2146	2141	2137	2132
4.7	2128	2123	2119	2114	2110	2105	2101	2096	2092	2088
4.8	2083	2079	2075	2070	2066	2062	2058	2053	2049	2045
4.9	2041	2037	2033	2028	2024	2020	2016	2012	2008	2004
5.0	2000	1996	1992	1988	1984	1980	1976	1972	1969	1965
5.1	1961	1957	1953	1949	1946	1942	1938	1934	1931	1927
5.2	1923	1919	1916	1912	1908	1905	1901	1898	1894	1890
5.3	1887	1883	1880	1876	1873	1869	1866	1862	1859	1855
5.4	1852	1848	1845	1842	1838	1835	1832	1828	1825	1821
5.5	1818	1815	1812	1808	1805	1802	1799	1795	1792	1789
5.6	1786	1783	1779	1776	1773	1770	1767	1764	1761	1757
5.7	1754	1751	1748	1745	1742	1739	1736	1733	1730	1727
5.8	1724	1721	1718	1715	1712	1709	1706	1704	1701	1698
5.9	1695	1692	1689	1686	1684	1681	1678	1675	1672	1669
6.0	1667	1664	1661	1658	1656	1653	1650	1647	1645	1642
6.1	1639	1637	1634	1631	1629	1626	1623	1621	1618	1616
6.2	1613	1610	1608	1605	1603	1600	1597	1595	1592	1590
6.3	1587	1585	1582	1580	1577	1575	1572	1570	1567	1565
6.4	1563	1560	1558	1555	1553	1550	1548	1546	1543	1541
6.5	1538	1536	1534	1531	1529	1527	1524	1522	1520	1517
6.6	1515	1513	1511	1508	1506	1504	1502	1499	1497	1495
6.7	1493	1490	1488	1486	1484	1481	1479	1477	1475	1473
6.8	1471	1468	1466	1464	1462	1460	1458	1456	1453	1451
6.9	1449	1447	1445	1443	1441	1439	1437	1435	1433	1431
7.0	1429	1427	1425	1422	1420	1418	1416	1414	1412	1410
7.1	1408	1406	1404	1403	1401	1399	1397	1395	1393	1391
7.2	1389	1387	1385	1383	1381	1379	1377	1376	1374	1372
7.3	1370	1368	1366	1364	1362	1361	1359	1357	1355	1353
7.4	1351	1350	1348	1346	1344	1342	1340	1339	1337	1335

Wavelength–Wavenumber Conversion Table (continued)

Wavelength, μm	Wavenumber, cm^{-1}									
	0	1	2	3	4	5	6	7	8	9
7.5	1333	1332	1330	1328	1326	1325	1323	1321	1319	1318
7.6	1316	1314	1312	1311	1309	1307	1305	1304	1302	1300
7.7	1299	1297	1295	1294	1292	1290	1289	1287	1285	1284
7.8	1282	1280	1279	1277	1276	1274	1272	1271	1269	1267
7.9	1266	1264	1263	1261	1259	1258	1256	1255	1253	1252
8.0	1250	1248	1247	1245	1244	1242	1241	1239	1238	1236
8.1	1235	1233	1232	1230	1229	1227	1225	1224	1222	1221
8.2	1220	1218	1217	1215	1214	1212	1211	1209	1208	1206
8.3	1205	1203	1202	1200	1199	1198	1196	1195	1193	1192
8.4	1190	1189	1188	1186	1185	1183	1182	1181	1179	1178
8.5	1176	1175	1174	1172	1171	1170	1168	1167	1166	1164
8.6	1163	1161	1160	1159	1157	1156	1155	1153	1152	1151
8.7	1149	1148	1147	1145	1144	1143	1142	1140	1139	1138
8.8	1136	1135	1134	1133	1131	1130	1129	1127	1126	1125
8.9	1124	1122	1121	1120	1119	1117	1116	1115	1114	1112
9.0	1111	1110	1109	1107	1106	1105	1104	1103	1101	1100
9.1	1099	1098	1096	1095	1094	1093	1092	1091	1089	1088
9.2	1087	1086	1085	1083	1082	1081	1080	1079	1078	1076
9.3	1075	1074	1073	1072	1071	1070	1068	1067	1066	1065
9.4	1064	1063	1062	1060	1059	1058	1057	1056	1055	1054
9.5	1053	1052	1050	1049	1048	1047	1046	1045	1044	1043
9.6	1042	1041	1040	1038	1037	1036	1035	1034	1033	1032
9.7	1031	1030	1029	1028	1027	1026	1025	1024	1022	1021
9.8	1020	1019	1018	1017	1016	1015	1014	1013	1012	1011
9.9	1010	1009	1008	1007	1006	1005	1004	1003	1002	1001
10.0	1000.0	999.0	998.0	997.0	996.0	995.0	994.0	993.0	992.1	991.1
10.1	990.1	989.1	988.1	987.2	986.2	985.2	984.3	983.3	982.3	981.4
10.2	980.4	979.4	978.5	977.5	976.6	975.6	974.7	973.7	972.8	971.8
10.3	970.9	969.9	969.0	968.1	967.1	966.2	965.3	964.3	963.4	962.5
10.4	961.5	960.6	959.7	958.8	957.9	956.9	956.0	955.1	954.2	953.3
10.5	952.4	951.5	950.6	949.7	948.8	947.9	947.0	946.1	945.2	944.3
10.6	943.4	942.5	941.6	940.7	939.8	939.0	938.1	937.2	936.3	935.5
10.7	934.6	933.7	932.8	932.0	931.1	930.2	929.4	928.5	927.6	926.8
10.8	925.9	925.1	924.2	923.4	922.5	921.7	920.8	920.0	919.1	918.3
10.9	917.4	916.6	915.8	914.9	914.1	913.2	912.4	911.6	910.7	909.9
11.0	909.1	908.3	907.4	906.6	905.8	905.0	904.2	903.3	902.5	901.7
11.1	900.9	900.1	899.3	898.5	897.7	896.9	896.1	895.3	894.5	893.7
11.2	892.9	892.1	891.3	890.5	889.7	888.9	888.1	887.3	886.5	885.7
11.3	885.0	884.2	883.4	882.6	881.8	881.1	880.3	879.5	878.7	878.0
11.4	877.2	876.4	875.7	874.9	874.1	873.4	872.6	871.8	871.1	870.3
11.5	869.6	868.8	868.1	867.3	866.6	865.8	865.1	864.3	863.6	862.8
11.6	862.1	861.3	860.6	859.8	859.1	858.4	857.6	856.9	856.2	855.4
11.7	854.7	854.0	853.2	852.5	851.8	851.1	850.3	849.6	848.9	848.2
11.8	847.5	846.7	846.0	845.3	844.6	843.9	843.2	842.5	841.8	841.0
11.9	840.3	839.6	838.9	838.2	837.5	836.8	836.1	835.4	834.7	834.0
12.0	833.3	832.6	831.9	831.3	830.6	829.9	829.2	828.5	827.8	827.1
12.1	826.4	825.8	825.1	824.4	823.7	823.0	822.4	821.7	821.0	820.3
12.2	819.7	819.0	818.3	817.7	817.0	816.3	815.7	815.0	814.3	813.7
12.3	813.0	812.3	811.7	811.0	810.4	809.7	809.1	808.4	807.8	807.1
12.4	806.5	805.8	805.2	804.5	803.9	803.2	802.6	801.9	801.3	800.6
12.5	800.0	799.4	798.7	798.1	797.4	796.8	796.2	795.5	794.9	794.3
12.6	793.7	793.0	792.4	791.8	791.1	790.5	789.9	789.3	788.6	788.0
12.7	787.4	786.8	786.2	785.5	784.9	784.3	783.7	783.1	782.5	781.9
12.8	781.3	780.6	780.0	779.4	778.8	778.2	777.6	777.0	776.4	775.8
12.9	775.2	774.6	774.0	773.4	772.8	772.2	771.6	771.0	770.4	769.8
13.0	769.2	768.6	768.0	767.5	766.9	766.3	765.7	765.1	764.5	763.9
13.1	763.4	762.8	762.2	761.6	761.0	760.5	759.9	759.3	758.7	758.2

Wavelength–Wavenumber Conversion Table (continued)

Wavelength, μm	Wavenumber, cm^{-1}									
	0	1	2	3	4	5	6	7	8	9
13.2	757.6	757.0	756.4	755.9	755.3	754.7	754.1	753.6	753.0	752.4
13.3	751.9	751.3	750.8	750.2	749.6	749.1	748.5	747.9	747.4	746.8
13.4	746.3	745.7	745.2	744.6	744.0	743.5	742.9	742.4	741.8	741.3
13.5	740.7	740.2	739.6	739.1	738.6	738.0	737.5	736.9	736.4	735.8
13.6	735.3	734.8	734.2	733.7	733.1	732.6	732.1	731.5	731.0	730.5
13.7	729.9	729.4	728.9	728.3	727.8	727.3	726.7	726.2	725.7	725.2
13.8	724.6	724.1	723.6	723.1	722.5	722.0	721.5	721.0	720.5	719.9
13.9	719.4	718.9	718.4	717.9	717.4	716.8	716.3	715.8	715.3	714.8
14.0	714.3	713.8	713.3	712.8	712.3	711.7	711.2	710.7	710.2	709.7
14.1	709.2	708.7	708.2	707.7	707.2	706.7	706.2	705.7	705.2	704.7
14.2	704.2	703.7	703.2	702.7	702.2	701.8	701.3	700.8	700.3	699.8
14.3	699.3	698.8	698.3	697.8	697.4	696.9	696.4	695.9	695.4	694.9
14.4	694.4	694.0	693.5	693.0	692.5	692.0	691.6	691.1	690.6	690.1
14.5	689.7	689.2	688.7	688.2	687.8	687.3	686.8	686.3	685.9	685.4
14.6	684.9	684.5	684.0	683.5	683.1	682.6	682.1	681.7	681.2	680.7
14.7	680.3	679.8	679.3	678.9	678.4	678.0	677.5	677.0	676.6	676.1
14.8	675.7	675.2	674.8	674.3	673.9	673.4	672.9	672.5	672.0	671.6
14.9	671.1	670.7	670.2	669.8	669.3	668.9	668.4	668.0	667.6	667.1
15.0	666.7	666.2	665.8	665.3	664.9	664.5	664.0	663.6	663.1	662.7
15.1	662.3	661.8	661.4	660.9	660.5	660.1	659.6	659.2	658.8	658.3
15.2	657.9	657.5	657.0	656.6	656.2	655.7	655.3	654.9	654.5	654.0
15.3	653.6	653.2	652.7	652.3	651.9	651.5	651.0	650.6	650.2	649.8
15.4	649.4	648.9	648.5	648.1	647.7	647.2	646.8	646.4	646.0	645.6
15.5	645.2	644.7	644.3	643.9	643.5	643.1	642.7	642.3	641.8	641.4
15.6	641.0	640.6	640.2	639.8	639.4	639.0	638.6	638.2	637.8	637.3
15.7	636.9	636.5	636.1	635.7	635.3	634.9	634.5	634.1	633.7	633.3
15.8	632.9	632.5	632.1	631.7	631.3	630.9	630.5	630.1	629.7	629.3
15.9	628.9	628.5	628.1	627.7	627.4	627.0	626.6	626.2	625.8	625.4
16.0	625.0	624.6	624.2	623.8	623.4	623.1	622.7	622.3	621.9	621.5
16.1	621.1	620.7	620.3	620.0	619.6	619.2	618.8	618.4	618.0	617.7
16.2	617.3	616.9	616.5	616.1	615.8	615.4	615.0	614.6	614.3	613.9
16.3	613.5	613.1	612.7	612.4	612.0	611.6	611.2	610.9	610.5	610.1
16.4	609.8	609.4	609.0	608.6	608.3	607.9	607.5	607.2	606.8	606.4
16.5	606.1	605.7	605.3	605.0	604.6	604.2	603.9	603.5	603.1	602.8
16.6	602.4	602.0	601.7	601.3	601.0	600.6	600.2	599.9	599.5	599.2
16.7	598.8	598.4	598.1	597.7	597.4	597.0	596.7	596.3	595.9	595.6
16.8	595.2	594.9	594.5	594.2	593.8	593.5	593.1	592.8	592.4	592.1
16.9	591.7	591.4	591.0	590.7	590.3	590.0	589.6	589.3	588.9	588.6
17.0	588.2	587.9	587.5	587.2	586.9	586.5	586.2	585.8	585.5	585.1
17.1	584.8	584.5	584.1	583.8	583.4	583.1	582.8	582.4	582.1	581.7
17.2	581.4	581.1	580.7	580.4	580.0	579.7	579.4	579.0	578.7	578.4
17.3	578.0	577.7	577.4	577.0	576.7	576.4	576.0	575.7	575.4	575.0
17.4	574.7	574.4	574.1	573.7	573.4	573.1	572.7	572.4	572.1	571.8
17.5	571.4	571.1	570.8	570.5	570.1	569.8	569.5	569.2	568.8	568.5
17.6	568.2	567.9	567.5	567.2	566.9	566.6	566.3	565.9	565.6	565.3
17.7	565.0	564.7	564.3	564.0	563.7	563.4	563.1	562.7	562.4	562.1
17.8	561.8	561.5	561.2	560.9	560.5	560.2	559.9	559.6	559.3	559.0
17.9	558.7	558.3	558.0	557.7	557.4	557.1	556.8	556.5	556.2	555.9
18.0	555.6	555.2	554.9	554.6	554.3	554.0	553.7	553.4	553.1	552.8
18.1	552.5	552.2	551.9	551.6	551.3	551.0	550.7	550.4	550.1	549.8
18.2	549.5	549.1	548.8	548.5	548.2	547.9	547.6	547.3	547.0	546.7
18.3	546.4	546.1	545.9	545.6	545.3	545.0	544.7	544.4	544.1	543.8
18.4	543.5	543.2	542.9	542.6	542.3	542.0	541.7	541.4	541.1	540.8
18.5	540.5	540.2	540.0	539.7	539.4	539.1	538.8	538.5	538.2	537.9
18.6	537.6	537.3	537.1	536.8	536.5	536.2	535.9	535.6	535.3	535.0
18.7	534.8	534.5	534.2	533.9	533.6	533.3	533.0	532.8	532.5	532.2
18.8	531.9	531.6	531.3	531.1	530.8	530.5	530.2	529.9	529.7	529.4
18.9	529.1	528.8	528.5	528.3	528.0	527.7	527.4	527.1	526.9	526.6

Wavelength–Wavenumber Conversion Table (continued)

Wavelength, μm	Wavenumber, cm^{-1}									
	0	1	2	3	4	5	6	7	8	9
19.0	526.3	526.0	525.8	525.5	525.2	524.9	524.7	524.4	524.1	523.8
19.1	523.6	523.3	523.0	522.7	522.5	522.2	521.9	521.6	521.4	521.1
19.2	520.8	520.6	520.3	520.0	519.8	519.5	519.2	518.9	518.7	518.4
19.3	518.1	517.9	517.6	517.3	517.1	516.8	516.5	516.3	516.0	515.7
19.4	515.5	515.2	514.9	514.7	514.4	514.1	513.9	513.6	513.3	513.1
19.5	512.8	512.6	512.3	512.0	511.8	511.5	511.2	511.0	510.7	510.5
19.6	510.2	509.9	509.7	509.4	509.2	508.9	508.6	508.4	508.1	507.9
19.7	507.6	507.4	507.1	506.8	506.6	506.3	506.1	505.8	505.6	505.3
19.8	505.1	504.8	504.5	504.3	504.0	503.8	503.5	503.3	503.0	502.8
19.9	502.5	502.3	502.0	501.8	501.5	501.3	501.0	500.8	500.5	500.3

[α], α	specific rotation and column head
>	above, more than
<	below, less than
∞	soluble in all proportions
ABBIA	*Archives of Biochemistry and Biophysics*
abs	absolute
ac	acid
Ac	acetyl
AC	Analytical Chemistry reference to spectra
ace, Ace	acetone
$aceD_6$	acetone deuterated
$aceF_6$	hexafluoro acetone
AcOEt	ethyl acetate
Ac_2O	acetic anhydride act
ACSAA	*Acta Chemica Scandivanica*
al	alcohol[1]
ALD	*The Aldrich Handbook of Organic Chemicals and Biochemicals*, Aldrich Chemical Co., Inc., New York; Aldrich Library of Infrared Spectra; Aldrich Library of Mass Spectra; Aldrich Chemical Co., Milwaukee, WI
ALDN	Aldermaston, *8 peak Index of Mass Spectra*, U.K.
alk	alkali
Am	amyl (pentyl)
AmOH	amyl alcohol
amor	amorphous
AMS	*Archives of Mass Spectral Data*, John Wiley & Sons, New York
ANCPA	*Annales de Chimie (Paris)*
anh	anhydrous
API	American Petroleum Institute spectral collection
aq	aqueous
ARKEA	*Arkiv foer Kemi*
as	asymmetric
atm	atmospheres
b	below
BCSJA	*Bulletin of the Chemical Society of Japan*
BIJOA	*Biochemical Journal*
bipym	bipyramidal
bk	black
bl	blue
bp	boiling point
BPSMA	*Bulletin de l'Academie Polonaise des Sciences*
br	brown
BSCFA	*Bulletin de la Societe Chimique de France*
BSCJA	*Bristol Chamber of Commerce Journal*
bt	bright
Bu	butyl
BuOH	butyl alcohol
bz, Bz	benzene
c	percentage concentration
ca	about
CA	*Chemical Abstracts*
CAS	Chemical Abstracts Service
CCCCA	*Collection of Czechoslovak Chemical Communications*
cello	cellosolve
CHBEA	*Chemische Berichte*
CHINA	*Chemistry and Industry*
chl, Chl	chloroform
CJCHA	*Canadian Journal of Chemistry*
co	columns
COB	Coblentz Society spectral collection
col	colorless
con, conc	concentrated
cor	corrected
COREA	*Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences*
ctc	carbon tetrachloride
cw	continuous wave
cy, cyhex	cyclohexane
cyD_{12}	cyclohexane deuterated
D	line in the emission spectrum of sodium (subscript), i.e., $[n]_D$
d, D	dextro
d	as column head, density
DANKA	*Doklady Akademii Nauk S.S.S.R.*
dec	decomposes
DFB	Dollish et al., *Characteristic Raman Frequencies of Organic Compounds*, John Wiley & Sons, New York
dil	diluted
diox	dioxane
dk	dark
dl, DL	racemic[2]
dlq	deliquescent
DMF	dimethyl formamide
$DMFd_6$	dimethyl formamide deuterated
DMS	Documentation of Molecular Spectroscopy spectral collection, Butterworth Scientific Publication, London WC2, England
DMSO	dimethyl sulfoxide
$DMSOd_6$	dimethyl sulfoxide deuterated
efl	efflorescent
Et	ethyl
eth	ether[3]
EtOH	ethyl alcohol
Et_2O	ethyl ether
exp	explodes
extrap	extrapolated
fl	flakes