

# 1 Introduction

## 1.1 General remarks

The present volume II/24 (published as five sub volumes II/24A, II/24B, II/24C, II/24D, and II/24E) is a supplement to and an extension of volume II/19 published in 1992-1994 and has been prepared on the understanding that it will be used in combination with II/4, II/6, II/14 and II/19. The reader will find helpful remarks on how to use the data listings, especially the definitions of the molecular constants, in front of each table.

Volume II/24 presents the spectroscopic data on diamagnetic and paramagnetic molecules as well as on molecular ions. For the diamagnetic species the publications up to the year of 1997 are included. The sub volumes for the paramagnetic species have been published later and cover the literature up to 2001. The spectroscopic information collected in this volume has been obtained principally from gas phase microwave measurements. In addition, gas phase data have been included derived from methods related to microwave spectroscopy by employing a coherent radiation source. These are molecular beam techniques, radio frequency spectroscopy, electron resonance spectroscopy, laser spectroscopy, double resonance and saturation techniques. Some other methods are considered if the accuracy of the derived molecular parameters is comparable to that of microwave spectroscopy owing to a good statistics in the analysis of data, and no microwave data are available. Examples would be Fourier infrared spectroscopy or laser induced fluorescence.

Internuclear distances are listed in the tables only for diatomic molecules and for some small open shell molecules. For all other polyatomic molecules the literature giving structural information has been cited.

A new comprehensive compilation of structural data is published in volume II/25 of the New Series of Landolt-Börnstein.

## 1.2 Review articles and tables

Some books treating recent developments in microwave spectroscopy are listed in 1.8, [1-7].

The Journal of Physical and Chemical Reference Data has published a series of tables of line frequencies, absorption intensities and molecular constants for diatomic [8], triatomic [9], selected polyatomic molecules and for molecules of particular interest in astrophysics. Some species of radicalic and ionic character are also included. The series started in 1972 and is continuing [10].

Since 1973 the Chemical Society (London) has regularly published a review on microwave spectroscopy [11].

Molecular constants from infrared spectroscopic data are currently published in Landolt-Börnstein New Series in volume II/20.

## 1.3 Arrangement of tables, substances and parameters

### 1.3.1 Arrangement of chapters and sections

The arrangement of data in Vols. II/4, II/6, and II/14 and II/19 is retained as far as possible. The data of molecules is listed in chapters 2 and 3.

In sections 2.2 through 2.5 the diamagnetic molecules are ordered according to the type of their respective spectrum as follows: Diatomic molecules (2.2), linear molecules (2.3), symmetric top molecules (2.4), and asymmetric top molecules (2.5). Molecules which are asymmetric only due to isotopic substitution are listed together with their parent species in 2.4. The tables include rotational constants, centrifugal distortion constants, rotation-vibration interaction constants, and  $\ell$ -type doubling constants. Some additional molecular constants obtained by microwave type methods have been listed as well. References to publications concerning the molecular structure are cited separately.

Tables 2.6 through 2.9 contain the dipole moments (2.6), nuclear quadrupole coupling constants (2.7), constants of hindered rotation (2.8) and magnetic interaction constants (2.9) of the molecules.

The literature used for chapter 2 is contained in separate sections of chapter 2 where for the reader's convenience the page where to find the appropriate reference section is indicated at the top of each page of the tables. The references are ordered according to the publication year followed by the three letters of the first author's name and in few cases by an additional running number. For each year the references are ordered alphabetically.

Chapter 3 contains the diatomic radicals (3.1) and the polyatomic radicals (3.2), where a radical is strictly defined here as a paramagnetic molecule. In chapter 3 the references are collected separately for each molecule.

The index of substances is provided in chapter 4, and terminates volume II/24. Chapters 2.1...2.4 are contained in the sub volume II/24A. Chapter 2.5 is presented in sub volume II/24B. Chapters 2.6...2.9 are given in sub volume II/24C. Chapter 3.2 is contained in the present sub volume II/24D2, chapter 3.1 will appear in II/24D1. Chapter 4 will be published in sub volume II/24E.

### 1.3.2 Arrangement within the sections of chapters 2 and 3

The arrangement of the columns within the sections of chapters 2 and 3 is similar to that in the previous volumes. The explanation of the symbols used in the tables is found under the subsection "Preliminary remarks" for each individual table. The ordering of the diamagnetic substances in each table of chapter 2 follows the early suggestion of Hill [12]. This means that the molecules are arranged in alphabetical order of the element symbols - with the exception of carbon and hydrogen atoms in organic compounds which are written first in that order. In this way, all organic substances are bound together between sum formulas starting with Br (if present) and those starting with Ca (if present). Deuterium is treated like hydrogen.

A typical series of substances according to Hill's system would be  $\text{AlF}_3$ ,  $\text{BCl}_3$ , ...,  $\text{B}_2\text{H}_6$ ,  $\text{CBrN}$ ,  $\text{CFN}$ ,  $\text{CHCl}_3$ ,  $\text{CH}_2\text{Cl}_2$ , ...,  $\text{CIN}$ ,  $\text{C}_2\text{H}$ , ...,  $\text{ClF}_5$ .

Note that the tables of diamagnetic molecules in the volumes II/4, II/6, and II/14, were organized in a different way.

The radicals (chapter 3) are not ordered strictly by Hill's system.

In this volume II/24, the ions are not collected separately but are included in the tables like the neutral molecules.

### 1.3.3 Explanation of the columns of the tables in chapters 2 and 3

In chapter 2, column 1 gives the running number of each molecule in the table. The numbers in the corresponding table of Vols. II/4, II/6, II/14, and II/19 are given below the running number.

Column 2 gives the structural formula of the molecule. The isotopic species are labeled with the isotopic numbers with the exception of the most abundant species, where the labels have been omitted.  $\text{C} = {}^{12}\text{C}$ ,  $\text{O} = {}^{16}\text{O}$ ,  $\text{S} = {}^{32}\text{S}$ ,  $\text{N} = {}^{14}\text{N}$ , etc.

The vibrational state of the molecule for which the listed constants were obtained is added (not in tables 2.9.2 and 2.9.3).

The next columns contain the values of the constants with which the table is concerned, and their references. Where several references are given, the first reference listed is the publication from which the numerical values were taken.

The last column of each table contains general remarks and values if necessary. This column also gives references to tables or diagrams which contain further information on the respective molecule. In tables 2.2 through 2.5 references are given in this column to all following tables and chapters. In tables 2.6 through 2.9 references are given only to tables 2.2 through 2.5. Thus all information given for each molecule may be reliably found by the use of tables 2.2 through 2.5.

In chapter 3, the complete set of molecular constants is collected often in front or behind a listing of reliable experimental transition frequencies separately for each species. Radicals require greatly differing angular momentum coupling schemes and therefore different kinds of effective hamiltonians for fitting spectra. Consequently, in contrast to chapter 2, the tabulations in chapter 3 show generally more individual character per molecule.

### 1.3.4 Notation of experimental errors

The error in a tabulated value is written as defined by the following equations (examples taken from LB. NS, Vol.II/7):

$$\begin{array}{rcl} 53479.72(25) \text{ cm}^{-1} & = & (53479.72 \pm 0.25) \text{ cm}^{-1} \\ 9.4(48) \text{ cm}^{-1} & = & (9.4 \pm 4.8) \text{ cm}^{-1} \\ 153.7754(13) \text{ pm} & = & (153.7754 \pm 0.0013) \text{ pm} \end{array}$$

Evidently the error given in parentheses on the left side applies to the last significant digits. According to international usage this notation normally indicates one standard deviation in molecular spectroscopy. Deviations thereof, if known from the literature, are specified in the tables.

## 1.4 Selection of data

For a molecule which was studied by several authors, the data of those authors are listed whose work (a) was the most complete (comparison of the data of a particular molecule), (b) was the most recent and (c) appeared to be the most accurate one. The work of other authors is cited in the references, but only the most recent paper of a particular research group is usually given. Data from dissertations and conference research reports were only included when no other publication could be located.

## 1.5 Abbreviations used for experimental methods

BMS	beam maser spectroscopy
EPR	electron paramagnetic resonance
FIR	far infrared spectroscopy
IR	infrared spectroscopy with or without laser
IRIRDR	infrared-infrared double resonance
IRMWDR	infrared-microwave double resonance
La	laser
LaSt	laser Stark spectroscopy
LC	level crossing spectroscopy
LIF	laser induced fluorescence
LMR	laser magnetic resonance
LRMW	low resolution microwave spectroscopy
MB	molecular beam electric/ magnetic resonance (sometimes for the state preparation and detection lasers are used)
MBE	molecular beam electric resonance
MBM	molecular beam magnetic resonance
MBRF	molecular beam radiofrequency spectroscopy
MBMW	molecular beam microwave and mm-wave spectroscopy

MODR	microwave optical double resonance
MOMRIE	microwave optical magnetic resonance induced by electrons
MW	microwave spectroscopy in the cm- and mm-wavelength region
OS	optical spectroscopy
QB	quantum beat spectroscopy
RFODR	radio frequency optical double resonance
RFIRDR	radio frequency infrared double resonance
RFMWDR	radio frequency microwave double resonance
SLS	saturated laser spectroscopy

Additional experimental techniques are indicated in the tables if necessary.

## 1.6 Selected fundamental constants and energy conversion factors

The determination of molecular constants from the measured frequencies of spectral lines needs best values of the fundamental constants. The “best values” improve with advancing techniques of measurement and changes in valuation. The recommended values listed in the following table are based on the publication by Mohr and Taylor [13].

### Recommended physical constants

Quantity	Symbol	Value	Units	
			SI	cgs
Speed of light	$c$	2.99792458 (exact)	$10^8 \text{ m s}^{-1}$	$10^{10} \text{ cm s}^{-1}$
Fine structure constant	$\alpha$	7.297352533 (27)	$10^{-3}$	$10^{-3}$
	$\alpha^{-1}$	137.03599976 (50)		
Electron charge	$e$	1.602176426(63)	$10^{-19} \text{ C}$	$10^{-20} \text{ emu}$
		4.803206 (15)		$10^{-10} \text{ esu}$
Planck's constant	$h$	6.62606876 (52)	$10^{-34} \text{ J s}$	$10^{-27} \text{ erg s}$
	$\hbar = h/2\pi$	1.054571596 (82)	$10^{-34} \text{ J s}$	$10^{-27} \text{ erg s}$
Avogadro's number	$N_A$	6.02214199 (47)	$10^{23} \text{ mol}^{-1}$	$10^{23} \text{ mol}^{-1}$
Atomic mass unit <sup>1)</sup>	$m_u = 1 \text{ u}$	1.66053873 (13)	$10^{-27} \text{ kg}$	$10^{-24} \text{ g}$
Proton rest mass	$m_p$	1.67262158 (13)	$10^{-27} \text{ kg}$	$10^{-24} \text{ g}$
Neutron rest mass	$m_n$	1.67492716 (13)	$10^{-27} \text{ kg}$	$10^{-24} \text{ g}$
Rydberg constant	$R_\infty$	1.0973731568549 (83)	$10^7 \text{ m}^{-1}$	$10^5 \text{ cm}^{-1}$
Bohr radius	$a_0$	5.291772083 (19)	$10^{-11} \text{ m}$	$10^{-9} \text{ cm}$
Bohr magneton	$\mu_B$	9.27400899 (37)	$10^{-24} \text{ J T}^{-1}$	$10^{-21} \text{ erg Gauss}^{-1}$
Nuclear magneton	$\mu_N$	5.05078317 (20)	$10^{-27} \text{ J T}^{-1}$	$10^{-24} \text{ erg Gauss}^{-1}$
Electron magnetic moment <sup>2)</sup>	$\mu_e$	9.28476362 (37)	$10^{-24} \text{ J T}^{-1}$	$10^{-21} \text{ erg Gauss}^{-1}$
Electron magnetic moment in Bohr magnetons <sup>2)</sup>	$\mu_e/\mu_B$	1.0011596521869 (41)		
Proton magnetic moment <sup>2)</sup>	$\mu_p$	1.410606633 (58)	$10^{-26} \text{ J T}^{-1}$	$10^{-23} \text{ erg Gauss}^{-1}$

<sup>1)</sup> The atomic mass unit is sometimes called 1 amu ( $= \frac{1}{12} m(^{12}\text{C}) = 1.6605402(10) \cdot 10^{-27} \text{ kg}$ ).

<sup>2)</sup> The modulus (length) of the vector is given (the direction is related to that of the spin, which is antiparallel for the electron and parallel for the proton).

These values yield the conversion factor  $I \cdot B$  relating rotational constant to moment of inertia:  
 $I \cdot B = 5.05379006(65) 10^5 \text{ amu } \text{\AA}^2 \text{ MHz}$ .

Note that authors may have used slightly variant values in their original work which is normally not corrected in the tables.

The following table for conversion between different energy scales may be used (uncertainties are all about 3 ppm, if needed, more accurate values may be calculated from the preceding table):

Energy conversion factors

	J	erg	eV	cm <sup>-1</sup>	cal	Hz
J	1	10 <sup>7</sup>	6.24151 · 10 <sup>18</sup>	5.03411 · 10 <sup>22</sup>	2.39006 · 10 <sup>-1</sup>	1.50919 · 10 <sup>33</sup>
erg	10 <sup>-7</sup>	1	6.24151 · 10 <sup>11</sup>	5.03411 · 10 <sup>15</sup>	2.39006 · 10 <sup>-8</sup>	1.50919 · 10 <sup>26</sup>
eV	1.60218 · 10 <sup>-19</sup>	1.60218 · 10 <sup>-12</sup>	1	8065.54	3.82931 · 10 <sup>-20</sup>	2.41799 · 10 <sup>14</sup>
cm <sup>-1</sup>	1.98645 · 10 <sup>-23</sup>	1.98645 · 10 <sup>-16</sup>	1.23984 · 10 <sup>-4</sup>	1	4.74763 · 10 <sup>-24</sup>	2.99792 · 10 <sup>10</sup>
cal	4.18400	4.18400 · 10 <sup>7</sup>	2.61144 · 10 <sup>19</sup>	2.10631 · 10 <sup>23</sup>	1	6.31445 · 10 <sup>33</sup>
Hz	6.62607 · 10 <sup>-34</sup>	6.62607 · 10 <sup>-27</sup>	4.13567 · 10 <sup>-15</sup>	3 33565 · 10 <sup>-11</sup>	1.58367 · 10 <sup>-34</sup>	1

## 1.8 References for 1

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