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**Numerical Data and Functional Relationships
in Science and Technology**

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aus Naturwissenschaften und Technik**

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Volume 14

Molecular Constants

**mostly from Microwave, Molecular Beam,
and Electron Resonance Spectroscopy**

Subvolume a



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LANDOLT-BÖRNSTEIN

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in Science and Technology

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Editor in Chief: K.-H. Hellwege

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Volume 14

Supplement to Volumes II/4 and II/6

Molecular Constants

mostly from Microwave, Molecular Beam,
and Electron Resonance Spectroscopy

Subvolume a

J. Demaison · A. Dubrulle · W. Hüttner · E. Tiemann

Editors: K.-H. Hellwege and A. M. Hellwege



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Darmstadt, Oktober 1982

Vorwort

Hiermit wird der erste Teilband, II/14a, des Bandes II/14 „Molekelkonstanten vorwiegend aus Messungen der Mikrowellen-, Molekularstrahl- und Elektronenresonanz-Spektroskopie“ vorgelegt, der ein Ergänzungsband von II/6 und damit der zweite Ergänzungsband von II/4 ist.

Die drei Bände II/4, II/6 und II/14 bilden zusammen eine vollständige, kritische Sammlung aller bis 1982 veröffentlichten Daten von Molekelkonstanten, die mit Hilfe der verschiedensten klassischen und neuen spektroskopischen Methoden gewonnen wurden.

Der Band II/14 wurde aus technischen Gründen geteilt. Der vorliegende Teilband II/14a enthält die allgemeine Einleitung und die Tabellen für die diamagnetischen Molekeln. Der Teilband II/14b, der die Strukturdiagramme der im Teilband a behandelten Molekeln, die Tabellen für die freien Radikale und das Substanzenverzeichnis enthält, wird anschließend erscheinen.

Für die zweiatomigen Molekeln sind wieder die Kernabstände zusammen mit den Molekelkonstanten angegeben. Für die Struktur der mehratomigen Molekeln sei – neben den im Teilband II/14b wieder zusammengestellten qualitativen Strukturzeichnungen, die die Richtung der verschiedenen tabellierten Größen illustrieren – auf den Band II/7 „Strukturdaten freier, mehratomiger Molekeln“ hingewiesen, der in einem der nächsten Jahre ergänzt werden wird.

Ein detailliertes Substanzenverzeichnis für alle drei Bände II/4, II/6 und II/14a,b am Ende des letzten Teilbandes, II/14b, ermöglicht das schnelle Auffinden der speziellen gesuchten Daten einer Substanz in einem dieser Bände.

Unser Dank gilt wieder den Autoren für ihre gründliche und schnelle Arbeit und für die angenehme Zusammenarbeit, sowie der „Sektion für Strukturdokumentation der Universität Ulm“, die ihr vollständiges Dokumentationsmaterial zur Verfügung stellte, aber auch der Landolt-Börnstein-Redaktion, insbesondere Frau R. Lettmann, für ihre zuverlässige Hilfe und dem Verlag für die übliche Sorgfalt bei der Fertigstellung des Bandes.

Auch dieser Band wird ohne finanzielle Hilfe von anderer Seite veröffentlicht.

Darmstadt, Oktober 1982

Die Herausgeber

Preface

This is the first subvolume, II/14a, of volume II/14 "Molecular Constants, mostly from Microwave, Molecular Beam and Electron Resonance Spectroscopy", which is the supplement to volume II/6 and thus the second supplement to volume II/4.

The three volumes II/4, II/6 and II/14 together present a complete compilation of the critically evaluated data on molecular constants from measurements with classical and modern spectroscopy which have been published until early 1982.

Volume II/14 had to be divided for technical reasons. The present subvolume contains the general introduction and the tables on diamagnetic molecules. Subvolume II/14b, containing the structure diagrams of the molecules treated in subvolume a, the tables on the free radicals, and the index of substances will appear subsequently.

The internuclear distances of diatomic molecules are supplemented together with the constants. The qualitative structure diagrams of polyatomic molecules illustrate the direction of various constants listed in the tables, while the complete tables of structure data may be found in volume II/7, "Structure Data of Free Polyatomic Molecules", which will be supplemented in one of the next years.

A detailed index of substances treated in the three volumes II/4, II/6, and II/14a, b is given at the end of subvolume II/14b and will help the user to locate quickly any special information on individual molecules in one of these volumes.

Our thanks are again due to the authors for their careful and quick work and for the agreeable cooperation, to the "Sektion für Strukturdokumentation der Universität Ulm" for making available their complete documentation material, and also to the editorial office, especially Mrs. R. Lettmann, for their reliable help and Springer Verlag for their usual care during the completion of the volume.

This subvolume is published without any outside financial support.

Darmstadt, October 1982

The Editors

Survey

Subvolume a

- 1 Introduction
- 2 Constants of diamagnetic molecules

Subvolume b

- 3 Figures
- 4 Constants of radicals
- 5 Appendix: Additions
- 6 Index of substances for Vol. II/4, II/6, and II/14

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3 Figures (J. DEMAISON, A. DUBRULLE)

4 Constants of radicals

4.1 Diatomic radicals (E. TIEMANN)

4.2 Polyatomic free radicals (J.M. BROWN)

5 Appendix: Additions

6 Index of substances for Vol. II/4, II/6, and II/14

Volume II/4 brings the spectroscopic data on molecules up to date transferring the publications up to and partly including 1981. 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, and double resonance techniques. Some other methods are considered if the accuracy of the derived molecular parameters is comparable to that of microwave spectroscopy and no microwave data are available. Examples would be Fourier transformed spectroscopy or electric deflection method.

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 compilation of ground state data has been published in 1976 in volume 1/7 of the New Series of Landolt-Börnstein and will be supplemented in the near future.

4.2 Review articles and tables

Books treating recent developments in microwave spectroscopy are listed in 1.1, [1-7].

The Journal of Physical and Chemical Reference Data has published a series of tables of line frequencies and molecular constants for diatomic molecules [8], triatomic molecules [9] and for molecules of particular interest in astrophysics.

A bibliography of experimental microwave spectroscopy (1945-1975) has been compiled in [10].

Since 1977 the Chemical Society (London) has regularly published a review of microwave spectroscopy [11].

1.3 Arrangement of tables, substances and parameters

1.3.1 Arrangement of chapters and sections

The arrangement of Vols. II/4 and II/6 is retained as far as possible. The data on molecules are listed in chapter 2 and those on radicals in chapter 4. In each section of chapter 2, a set of related constants and physical quantities is tabulated for all of the molecules included, whereas in chapter 4 all relevant constants and physical quantities of each radical are listed together in individual tables.

In section 2.2 through 2.5 the molecules (radicals are included with reference to chapter 4) are ordered according to the type of their respective rotational spectrum as follows: 1) 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 K -type coupling 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.

In chapter 3, structural diagrams of various molecules can be found.

The literature used for chapter 2 is contained in separate sections of chapter 2, collected by the various authors and concerning their own contributions. 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 first author's name and in few cases, by an additional running number. For each year the references are ordered alphabetically.

In chapter 4 the data from investigations of radical cations and electronic states of molecules have been compiled. The diatomic radicals are listed in 4.1, the polyatomic ones in 4.2.

Chapter 5 consists of additional data which came in our attention after the page proof of the tables.

Chapter 6 gives the index of substances. If this are running numbers for each molecule in all the tables in which the molecule appears both in the present volume II/4 and in the previous volumes II/4 and II/6, inorganic

1 Introduction

1.1 General remarks

The present volume II/14 (published as two subvolumes II/14a and II/14b) is a supplement to and an extension of volume II/6 published in 1974 and has been prepared on the understanding that it will be used in combination with II/4 and II/6. The preliminary remarks of II/4 apply also to this supplement and are not repeated. The remarks relating to each table and the definitions of the listed constants, however, are rewritten in the present volume. Data on a particular substance can be found through the common index at the end of sub-volume II/14b.

Volume II/14 brings the spectroscopic data on molecules up to date considering the publications up to and partly including 1981. 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, and double resonance techniques. Some other methods are considered if the accuracy of the derived molecular parameters is comparable to that of microwave spectroscopy and no microwave data are available. Examples would be Fourier infrared spectroscopy or electric deflection method.

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 compilation of structural data has been published in 1976 in volume II/7 of the New Series of Landolt-Börnstein and will be supplemented in the near future.

1.2 Review articles and tables

Some books treating recent developments in microwave spectroscopy are listed in 1.7, [1-7].

The Journal of Physical and Chemical Reference Data has published a series of tables of line frequencies and molecular constants for diatomic molecules [8], triatomic molecules [9] and for molecules of particular interest in astrophysics.

A bibliography of experimental microwave spectroscopy (1945-1975) has been compiled in [10].

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

1.3 Arrangement of tables, substances and parameters

1.3.1 Arrangement of chapters and sections

The arrangement of Vols. II/4 and II/6 is retained as far as possible. The data on molecules are listed in chapter 2 and those on radicals in chapter 4. In each section of chapter 2, a set of related constants and physical quantities is tabulated for all of the molecules included, whereas in chapter 4 all measured constants and physical quantities of each radical are listed together in individual tables.

In section 2.2 through 2.5 the molecules (radicals are included with references to chapter 4) are ordered according to the type of their respective rotational 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 *l*-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.

In chapter 3, structural diagrams of various molecules are to be found.

The literature used for chapter 2 is contained in separate sections of chapter 2, collected by the various authors and concerning their own contributions. 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 first author's name and in few cases, by an additional running number. For each year the references are ordered alphabetically.

In chapter 4 the data from investigations of radicals (non- $^1\Sigma$ electronic states of molecules) have been compiled. The diatomic radicals are listed in 4.1, the polyatomic ones in 4.2.

Chapter 5 consists of additional data which came to our attention after the page proof of the tables.

Chapter 6 gives the index of substances. It lists the running numbers for each molecule in all the tables in which the molecule appears both in the present volume II/14 and in the previous volumes II/4 and II/6. Inorganic

(not containing carbon) and organic (containing carbon) substances are listed in separate sections and arranged alphabetically according to their alphabetically ordered gross formula.

Chapters 1 and 2 are contained in the present subvolume II/14a.

Chapters 3, 4, 5 and 6 will be published subsequently in subvolume II/14b.

1.3.2 Arrangement within the sections of chapter 2

The arrangement of the columns within the sections of chapter 2 is the same as in chapter 2 of Vols. II/4 and II/6. The explanation of the symbols used in the tables is found under the subsection "Preliminary remarks" for each individual table. In order to favour comparison between similar molecules, the ordering of molecules in a particular table follows a specific pattern. A brief explanation or survey at the end of the subsection "Preliminary remarks" of each table gives the ordering procedure adopted for the compounds. A particular molecule can easily be found with the help of the index of substances, chapter 6 (Subvolume II/14b).

1.3.3 Explanation of the columns of the tables 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 and II/6 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: C=¹²C, O=¹⁶O, S=³²S, N=¹⁴N, 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 reliably be found by use of either tables 2.2 through 2.5, or the index of substances in chapter 6 (Subvolume II/14b).

1.3.4 Arrangements within the sections of chapter 4

The data are compiled in individual tables for each radical. The diatomic radicals are treated in section 4.1, the polyatomic ones in 4.2.

In sections 4.1 and 4.2 radicals are arranged in subsections according to the electronic states with running numbers in each subsection. The data for each molecule are contained in two tables. The first table lists the observed frequencies and their assignment to specific transitions as indicated by the various quantum numbers (electronic, vibrational, rotational, hyperfine, and parity). The second table gives all constants and parameters which were available.

The constants and parameters used in the tables are defined in a short introduction preceding the tables of each subsection. The literature is given for each radical separately.

1.3.5 Errors

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

$$3.478(21) \text{ \AA} = (3.478 \pm 0.021) \text{ \AA}$$

$$13.4(21) \text{ \AA} = (13.4 \pm 2.1) \text{ \AA}$$

$$119.3(2) \text{ deg} = (119.3 \pm 0.2) \text{ \AA}$$

Evidently the error given in parentheses on the left side applies to the last significant digits.

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 reliable one. The work of other authors is cited in the references, but only the most recent paper of a particular research group is 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
ED	electric deflection method
EPR	electron paramagnetic resonance
FIR	far infrared spectroscopy [Sections 2.3, 2.4, 2.5, 2.6.2, 2.6.3, 2.7.2, 2.7.3, 2.8] Fourier infrared spectroscopy [Sections 2.2, 2.6.1, 2.7.1, 2.9.1]
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 (or MBER)	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
RF/DR	radio frequency optical double resonance
RFIRDR	radio frequency infrared double resonance
RFMWDR	radio frequency microwave double resonance
SLs	saturated laser spectroscopy

1.6 Selected fundamental constants and conversion factors

The calculation 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 taken from the publication by Cohen and Taylor [12].

Recommended physical constants

Quantity	Symbol	Value	Units	
			SI	cgs
Velocity of light	c	2.99792458 (12)	10^8 m sec^{-1}	$10^{10} \text{ cm sec}^{-1}$
Fine-structure constant	α	7.2973506 (60)	10^{-3}	10^{-3}
	α^{-1}	137.03604 (11)		
Electron charge	e	1.6021892 (46)	10^{-19} C	10^{-20} emu
		4.803242 (14)		10^{-10} esu
Planck's constant	h	6.626176 (36)	$10^{-34} \text{ J} \cdot \text{sec}$	$10^{-27} \text{ erg} \cdot \text{sec}$
	$\hbar = h/2\pi$	1.0545887 (57)	$10^{-34} \text{ J} \cdot \text{sec}$	$10^{-27} \text{ erg} \cdot \text{sec}$
Avogadro's number	N	6.022045 (31)	$10^{26} \text{ kmol}^{-1}$	10^{23} mol^{-1}
Atomic mass unit	amu	1.6605655 (86)	10^{-27} kg	10^{-24} g
Electron rest mass	m_{el}	9.109534 (47)	10^{-31} kg	10^{-28} g
		5.4858026 (21)	10^{-4} amu	10^{-4} amu
Proton rest mass	m_p	1.6726485 (86)	10^{-27} kg	10^{-24} g
		1.007276470 (11)	amu	amu
Neutron rest mass	m_n	1.6749543 (86)	10^{-27} kg	10^{-24} g
		1.008665012 (37)	amu	amu

(continued)

Recommended physical constants (continued)

Quantity	Symbol	Value	Units	
			SI	cgs
Electron charge to mass ratio	e/m_{el}	1.7588047 (49) 5.272764 (15)	$10^{11} \text{ C kg}^{-1}$	10^7 emu g^{-1} $10^{17} \text{ esu g}^{-1}$
Rydberg constant	R_{∞}	1.097373177 (83)	10^7 m^{-1}	10^5 cm^{-1}
Bohr radius	a_0	5.2917706 (44)	10^{-11} m	10^{-9} cm
Classical electron radius	r_0	2.8179380 (70)	10^{-15} m	10^{-13} cm
Electron magnetic moment in Bohr magnetons	μ_{el}/μ_B	1.0011596567 (35)		
Bohr magneton	μ_B	9.274078 (36)	$10^{-24} \text{ J T}^{-1}$	$10^{-21} \text{ erg Gauss}^{-1}$
Nuclear magneton	μ_n	5.050824 (20)	$10^{-27} \text{ J T}^{-1}$	$10^{-24} \text{ erg Gauss}^{-1}$
Electron magnetic moment	μ_{el}	9.284832 (36)	$10^{-24} \text{ J T}^{-1}$	$10^{-21} \text{ erg Gauss}^{-1}$
Proton magnetic moment in Bohr magnetons	μ_p/μ_B	1.521032209 (16)	10^{-3}	10^{-3}
Proton magnetic moment	μ_p	1.4106171 (55)	$10^{-26} \text{ J T}^{-1}$	$10^{-23} \text{ erg Gauss}^{-1}$

These values yield the conversion factor $I \cdot B$:

$$I [\text{amu } \text{\AA}^2] \cdot B [\text{MHz}] = 5.0537905(85) \cdot 10^5 \text{ amu } \text{\AA}^2 \text{ MHz.}$$

In fact a slightly different value of this conversion factor is very often used:

$$I B = 505376 \text{ amu } \text{\AA}^2 \text{ MHz.}$$

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^{-1}	$\text{cal} \cdot \text{mol}^{-1}$	Hz
J	1.0	10^7	$6.24146 \cdot 10^{18}$	$5.03404 \cdot 10^{22}$	$1.43834 \cdot 10^{23}$	$1.50916 \cdot 10^{33}$
erg	10^{-7}	1.0	$6.24146 \cdot 10^{11}$	$5.03404 \cdot 10^{15}$	$1.43834 \cdot 10^{16}$	$1.50916 \cdot 10^{26}$
eV	$1.60219 \cdot 10^{-19}$	$1.60219 \cdot 10^{-12}$	1.0	8065.48	$2.30450 \cdot 10^4$	$2.41797 \cdot 10^{14}$
cm^{-1}	$1.98648 \cdot 10^{-23}$	$1.98648 \cdot 10^{-16}$	$1.23985 \cdot 10^{-4}$	1.0	2.85724	$2.99793 \cdot 10^{10}$
$\text{cal} \cdot \text{mol}^{-1}$	$6.95246 \cdot 10^{-24}$	$6.95246 \cdot 10^{-17}$	$4.33934 \cdot 10^{-5}$	$3.49989 \cdot 10^{-1}$	1.0	$1.04851 \cdot 10^{10}$
1 Hz	$6.62620 \cdot 10^{-34}$	$6.62620 \cdot 10^{-27}$	$4.13571 \cdot 10^{-15}$	$3.33564 \cdot 10^{-11}$	$9.53731 \cdot 10^{-11}$	1.0

1.7 References

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2 Constants of diamagnetic molecules

2.1 Survey

Rotational constants etc.	Table 2.2...2.5
Dipole moments	Table 2.6
Quadrupole coupling constants	Table 2.7
Hindered rotation	Table 2.8
Magnetic constants	Table 2.9

2.2 Diatomic molecules

Rotational constants, centrifugal distortion constants, rotation-vibration interaction constants, Dunham energy coefficients, parameters of the breakdown of the Born-Oppenheimer approximation, and equilibrium internuclear separations

2.2.1 Preliminary remarks

1. Introduction

This table contains the molecular parameters which describe the rotational energy in a specific electronic state and in different vibrational states. Values are given only for molecules the electronic state of which is assigned to $^1\Sigma^+$ or O^+ . For other electronic states of the same molecules or for radicals references to tables 2.6, 2.7 and 4 are given.

Most of the molecular constants used are explained in Section 2.2.1 of Vol. II/6 Landolt-Börnstein, New Series. Only a brief supplement will be presented here to introduce some new parameters.

In all disciplines of molecular spectroscopy, the rotational-vibrational energy is described by a power series of $J(J+1)$ and $(v+1/2)$, where J and v are the rotational and vibrational quantum numbers, respectively. As parameters, the Dunham notation Y_{jk} or the original spectroscopic notation $B_e^{\text{spec}}, \alpha_e^{\text{spec}}, \dots, \omega_e^{\text{spec}}, \dots$ are in use. But in both notations, the values of these parameters are obtained by fitting the same formula to the measured spectral line positions. Therefore both types of constants are the same and only disagree by the signs $\pm$ which were originally defined for the series $B_e, \alpha_e, \dots$. The following relations are given as examples:

$$\begin{aligned} Y_{10} &= \omega_e^{\text{spec}} \\ -Y_{20} &= \omega_e \chi_e^{\text{spec}} \\ Y_{01} &= B_e^{\text{spec}} \\ -Y_{11} &= \alpha_e^{\text{spec}} \quad \text{etc.} \end{aligned}$$

The upper script "spec" is written in the case of the phenomenological parameters in order to distinguish between these and the physically defined constants B_e and ω_e :

$$B_e^{\text{cor}} = \frac{h}{8\pi^2 \mu_{\text{red}} (r_e^{\text{cor}})^2} \quad \text{rotational constant for equilibrium configuration } e$$

$$\omega_e = 2\sqrt{a_0 \cdot B_e^{\text{cor}}} \quad \text{harmonic vibrational constant}$$

which are both related to the potential $U(r)$ for the motion of the two atoms within the Born-Oppenheimer approximation and where

h Planck's constant

μ_{red} reduced atomic mass of the molecule

r_e^{cor} equilibrium internuclear distance corrected for the breakdown of the Born-Oppenheimer approximation

$a_0 \cdot 2$ second derivative of $U(r)$ with respect to $\xi = \frac{r-r_e}{r_e}$ at $\xi=0$

a_0 is proportional to the harmonic force constant.

As reviewed by Watson [1] the breakdown of the Born-Oppenheimer approximation can be accounted for by the following formula in the case of the rotational constant Y_{01} for a molecule AB:

$$Y_{01} = B_e^{\text{cor}} \left[1 - 2m_e \left(\frac{d_A}{M_A} + \frac{d_B}{M_B} \right) \right] \quad (1)$$

where

m_e mass of the electron

$M_{A,B}$ mass of a specific isotope of atom A or B

$d_{A,B}$ phenomenological parameters for the adiabatic and non-adiabatic Born-Oppenheimer corrections of atom A or B including the usual Dunham correction.

Similar relations are valid for the other Dunham parameters Y_{ik} (compare Watson [1] and Bunker [2]) but are not used to describe the observed spectra. The IR-spectrum of CO is the only exception. The parameters d_A, d_B can be determined by isotopic substitution of both atoms separately. An overall fit of all molecular isotopes observed will give the most reliable set of parameters, which is included in the tables and from which molecular constants of all isotopes can be calculated with high precision by using simple mass relations (compare [3]). If data exist only for individual isotopes of one molecule in the literature, it is all included in the tables.

Sometimes the Born-Oppenheimer correction is described with δ -parameters (compare the definition in Vol. II/6 and [4]), which do not take into account the different behavior of atom A and B. Therefore this data should be recalculated to get comparable information.

2. Explanations of the columns in the tabulation

Column	Parameters	Definitions
1	Nr. 6-Nr.	serial number of the diatomic molecule used in all tables of this book the second number represents the serial number in table 2.2 of Vol. II/6 Landolt-Börnstein, New Series
2	B [MHz] B_e $B_{0,1,2,\dots}$ Y_{01} [MHz]	rotational constant for the equilibrium configuration e , compare column 3 for the vibrational state $v=0, 1, 2, \dots$, compare column 3 Dunham's rotational constant
3	D [kHz] D_e $D_{0,1,2,\dots}$ Y_{02} [kHz] β_e [kHz] Y_{12} [kHz] H [kHz] Y_{03} [kHz] H_e	centrifugal distortion constant for the equilibrium configuration e for the vibrational state $v=0, 1, 2, \dots$, Dunham's centrifugal distortion constant higher-order rotation-vibration interaction constant Dunham's higher-order rotation-vibration interaction constant higher-order centrifugal distortion constant Dunham's higher-order centrifugal distortion constant
4	α, γ [MHz] Y_{11} [MHz] Y_{21} [MHz] Y_{31} [MHz]	α_e, γ_e rotation-vibration interaction constants Dunham energy coefficients for vibration-rotation interaction
5	Ref.	references for columns 2...4, 8, 9
6	Meth. MW MB IR MODR	method of measurement used in the given reference corresponding to the preceding quoted values microwave spectroscopy molecular beam resonance experiment-electric or magnetic resonance infrared with lasers microwave optical double resonance
7	$a_0, a_1, a_2, a_3, \dots$ d_A, d_B δ_1, δ_2 $Y_{10}, Y_{20}, \dots$	potential constants for a power series of $U(r)$ according to $\xi = \frac{r - r_e}{r_e}$ parameters of the breakdown of the Born-Oppenheimer approximation vibrational parameters determined from MW-measurements or high precision IR-spectroscopy

Column	Parameters	Definitions
8	r [Å]	internuclear distance; see also 3.
	r_e	equilibrium value of the internuclear distance calculated from $Y_{01} = h/(8\pi^2 \mu_{\text{red}} r_e^2)$
	$\tilde{r}_e$	equilibrium value of the internuclear distance calculated from B_e , subtracted the Dunham-correction δ_3 , compare Eq. (4) of Vol. II/6 Landolt-Börnstein, New Series
	r_e^{cor}	equilibrium value of the internuclear distance calculated from B_e^{cor} , compare Eq. (1)
9		references to following tables

All measured or derived values Y_{ik} —or the equivalent constants as defined in Vol. II/6 Landolt-Börnstein, New Series—, which are listed in the quoted references, are also tabulated, even when they are not indicated in the column headings of the table.

List of abbreviations for indexes:

cor corrected =corrected to allow for a treatment of the molecule different from the Born-Oppenheimer approximation

der derived =derived from the measured values by simple interrelations

e equilibrium =symbol representing the equilibrium configuration

e electron

el electron, electronic

ev evaluated =evaluated with the use of experimental values from other spectroscopic regions

n nuclear

p proton

red reduced.

3. Conversion factors

For the calculation of the internuclear distance different conversion factors $h/(8\pi^2 m_0)$ (m_0 =atomic mass unit) are used in the literature. Throughout these tables the value

$$B \text{ [MHz]} \cdot I \text{ [amu Å}^2\text{]} = 505391 \text{ MHz amu Å}^2$$

will be adopted. For any theoretical model interpretation, it seems unimportant which of the existing conversion factors is used at the moment, because the different values will change the r_e -parameters by an amount of about $2 \cdot 10^{-5}$ only. The errors shown for r_e are the experimental errors neglecting the uncertainty of the conversion factor. The relative atomic masses for the calculation of the Born-Oppenheimer approximation are usually taken from latest published atomic mass tables [5]. But there are several exceptions because the authors of the original publication used other values for the masses. In order to get full consistency for all data the whole fitting procedure would have to be repeated. But this would lead to slight changes only in the molecular parameters and will not alter the physical interpretation. On the other hand for predicting spectral lines with high reliability the reader should use the originally adopted mass values and is advised to refer to the original work.

For conversion of cm^{-1} to Hz the value 299792458 m/s is used for the speed of light.