

General Information

Volume Title	Editor/Authors	Preface
Publication Data	Table of Contents	Survey
Substance Index	Introduction	Symbols

Survey on Structure Data of Free Molecules in electronic ground state and in electronically excited states

Polyatomic molecules in Vol.	II/25		
Molecules without C atoms	Subvolume	A	
Molecules with C atoms	Subvolumes	B (C ₁ , C ₂), C (C ₃ , C ₄), D (C ₅ – C ₆₀)	
Diatomic molecules in Vols.	II/6	II/14a, b	II/19a, b, c, d
Diamagnetic molecules	Section 2.2	Section 2.2, Appendix	Sections 2.2, 2.1.6, 2.7.1, 1.9.1
Free radicals	Section 4.1	Section 4.1	Sections 3.1, 3.2

List of symbols in II/25

A, B, C	Rotational constants (see 1.2.1)
$\tilde{X}, \tilde{A}, \tilde{B}, \tilde{C}$	Labels for electronic states, ground state labelled \tilde{X}
$\tilde{a}, \tilde{b}, \tilde{c}, \dots$	Labels for excited electronic states of spin-multiplicity differing from that of the ground state \tilde{X}
r	Internuclear distance (X–Y = bond distance, X...Y = nonbonded distance)
r_e	Distance between equilibrium nuclear positions
r_{av}, r_z, r_α^0	Distance between average nuclear positions (ground vibrational state, $v_1 = v_2 \dots = 0$)
r_α	Distance between average nuclear positions (thermal equilibrium)
r_0	Distance between effective nuclear positions derived from rotational constants of zero-point vibrational level ($v_1 = v_2 \dots = 0$)
r_s	Distance between effective nuclear positions derived from isotopic differences in rotational constants
r_m	Distance between effective nuclear positions derived from the mass-dependence method of Watson
r_g	Thermal average value of internuclear distance
r_a	Constant argument in the molecular term, Eq. (8), see Table 1.3.3
f, k	Force constant for a weakly bound complex
θ	Bond angle; for indices, see r . For example, θ_e, θ_z and θ_α represent angles defined by a set of three nuclear positions, equilibrium, average (ground vibrational state) and average (thermal equilibrium), respectively, and θ_a by a set of three internuclear distances r_a . Some electron diffraction papers report distances as r_g and angles as θ_α or θ_z .
ν	Vibrational wavenumber for a weakly bound complex

List of abbreviations in II/25

CEI	Coulomb explosion imaging	ZEKE	Zero kinetic energy
ED	Electron diffraction		photoelectron spectroscopy
IR	Infrared spectroscopy	ac	anticlinal
LIF	Laser induced fluorescence	ap	antiperiplanar
LMR	Laser magnetic resonance	ax	axial
MW	Microwave spectroscopy	b	bending vibrational mode
NMR	Nuclear magnetic resonance	b	bridge
PES	Photoelectron spectroscopy	cm	center of mass
Ra	Raman spectroscopy	eq	equatorial
REMPI	Resonance enhanced multiphoton ionization	s	stretching vibrational mode
		sc	synclinal
TPI	Two photon ionisation (spectroscopy)	sp	synperiplanar
UV	Ultraviolet spectroscopy	t	terminal

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Some of the group names have been changed according to a better description of their contents.

Landolt-Börnstein

Numerical Data and Functional Relationships in Science and Technology

New Series / Editor in Chief: W. Martienssen

Group II: Molecules and Radicals

Volume 25

Structure Data of Free Polyatomic Molecules

Subvolume C

Molecules containing Three or Four Carbon Atoms

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Springer

ISSN 1615-1852 (Molecules and Radicals)

ISBN 3-540-66774-1 Springer-Verlag Berlin Heidelberg New York

Library of Congress Cataloging in Publication Data:

Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology, New Series.

Editor in Chief: W. Martienssen

Vol. II/25C: Edited by K. Kuchitsu

At head of title: Landolt-Börnstein. Added t.p.: Numerical data and functional relationships in science and technology.

Springer-Verlag, Berlin Heidelberg New York 2000.

Includes bibliographies.

1. Physics – Tables. 2. Chemistry – Tables. 3. Engineering – Tables.

I. Börnstein, Richard (1852-1913). II. Landolt, Hans (1831-1910)

III. Physikalisch-chemische Tabellen. IV. Numerical Data and Functional Relationships in Science and Technology.

QC 61.23 502'.12 62-53136

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Printed in Germany

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Typesetting: Authors and Redaktion Landolt-Börnstein, Darmstadt

Printing: Computer to plate, Mercedes-Druck, Berlin

Binding: Lüderitz & Bauer, Berlin

SPIN: 1068 8787 63/3020-5 4 3 2 1 0 – Printed on acid-free paper

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^{*}) This description holds also for the contribution to volume II/25B.

Preface

The first volume of this series, "Structure Data of Free Polyatomic Molecules" published in 1976 as II/7, contained all structural data for free polyatomic molecules in the ground state and in excited electronic states published in journals between 1960 and June 1974.

Three supplementary volumes have since been published: II/15 (July 1974-1984) in 1987, II/21 (1985-1989) in 1992, and II/23 (1990-1993) in 1995.

The present volume II/25 consists of four subvolumes, each containing all the structural data published in 1994 and 1995, with a few exceptions published afterwards. In addition, all the data listed in the previous volumes are also incorporated after appropriate revisions. Therefore, this volume is a comprehensive list of data for more than 3500 free polyatomic molecules published between 1960 to 1995 inclusive:

Subvolume **A**: 877 molecules containing no carbon atoms.

Subvolume **B**: 992 molecules containing one or two carbon atoms

Subvolume **C**: 893 molecules containing three or four carbon atoms

Subvolume **D**: about 1000 molecules containing five or more carbon atoms

Each subvolume contains an electronic version on CD-ROM (Portable Data Files, PDF 3.0, the Acrobat reader 3.0 with full text search engine for a variety of computer platforms is included).

All experimental methods for the determination of quantitative structural data of free molecules have been considered: microwave, infrared, Raman, electronic and photoelectron spectroscopy and related spectroscopic methods as well as electron diffraction. All data obtained by these methods have been critically evaluated and compiled. The data are presented separately for each molecule, together with original references and in many cases with computer-drawn figure(s) carefully prepared by Dr. N. Vogt.

My sincere thanks are due to the Editor in Chief, Professor W. Martienssen, for his thoughtful guidance and to all authors of the present volume for their thorough and intensive work and for close cooperation; to Dr. B. Mez-Starck, Freiburg, and Sektion für Spektren- und Struktur-dokumentation, Universität Ulm, for their valuable assistance and support; and to Springer-Verlag, especially Dr. R. Poerschke, for continual support and care. I greatly appreciate the expert help of Professors K. Hata and M. Nakahara in improving the nomenclature, Professor D.W.H. Rankin in reading the manuscript data sheets and Dr. D.A. Ramsay with checking the English text.

I am also grateful to the former Editors in Chief of Landolt-Börnstein and the former Volume Editors for II/7 and 15: Professor K.-H. Hellwege, Dr. A.M. Hellwege and Professor O. Madelung, for their initiative and permanent support, to the coauthors of the preceding volumes II/7, 15 and 21: Drs. J.H. Callomon, W.J. Lafferty, A.G. Maki and C.S. Pote, for their expert contributions, and to the Redaktion Landolt-Börnstein Darmstadt for their valuable help, especially Dr. T. Schneider for his reliable and careful assistance in preparation of this volume.

Sakado, July 2000

The Editor

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