

Ions by V.G. Pal'chikov and V.P. Shevelko (Springer, Berlin, Heidelberg 1995) and *Atoms and Their Spectroscopic Properties* by V.P. Shevelko (Springer, Berlin, Heidelberg 1997). It is intended for research students and specialists dealing with chemical physics, astrophysics, controlled plasma fusion, spectroscopy and related fields of atomic and molecular physics.

The authors acknowledge very much the help of Ludmila Khristenko and Natalia Kozulina in preparing the manuscript.

Moscow
December 1997

S.V. Khristenko
A.I. Maslov
V.P. Shevelko

Contents

1 Molecular Structure	1
1.1 Classification of Chemical Bonds and Molecular Terms	1
1.1.1 Electronic Energy Levels	3
1.1.2 Vibrational Energy Levels	4
1.1.3 Rotational Energy Levels	6
1.2 Coupling Schemes	8
1.3 Quantum Chemistry Methods	9
1.4 Equilibrium Form of Molecules	15
1.5 Potential-Energy Curves	16
1.6 Corrections to the Electronic Structure	17
1.6.1 Hyperfine Interaction and Isotope Effect	17
1.6.2 Relativistic Effects	18
2 Spectroscopic and Geometrical Constants of Molecules	20
2.1 Constants of Diatomic Molecules	20
2.2 Fundamental Vibrational Frequencies of Polyatomic Molecules ..	27
2.3 Rotational Constants and Geometrical Parameters of Polyatomic Molecules	32
3 Energy Constants of Molecules	39
3.1 Bond Dissociation Energies	39
3.2 Ionization Potentials	51
3.3 Electron Affinities	51
3.4 Proton Affinities	64
4 Electrical Properties of Molecules	71
4.1 Dipole Moments	71
4.2 Multipole Moments	78
4.3 Molecular Polarizabilities	82
5 Molecular Spectra	87
5.1 Types of Transitions and Selection Rules	87
5.2 Oscillator Strengths and Transition Probabilities	89
5.2.1 Rotational Spectra	89
5.2.2 Vibrational and Vibrational-Rotational Spectra	90
5.2.3 Rovibronic Spectra	91

5.2.4 Franck-Condon Factors	97
5.3 Photoionization	112
6 Collisions of Molecules with Electrons	122
6.1 Basic Approaches	122
6.2 Types of Collision Processes	126
6.3 Elastic Scattering	127
6.4 Excitation of Molecules by Electron Impact	138
6.4.1 Rotational Excitation	138
6.4.2 Vibrational Excitation	144
6.4.3 Electronic Excitation	149
6.4.4 Resonance Processes	153
6.5 Dissociation and Dissociative Attachment	154
6.5.1 Dissociative Processes	155
6.6 Ionization by Electron Impact	161
6.7 Electron-Ion Recombination and Electron Attachment	167
7 Interatomic Potentials	175
7.1 Interaction Constants	175
7.1.1 Van-der-Waals Interaction	176
7.1.2 The van-der-Waals Equation of State	182
7.1.3 The Lennard-Jones Potential	182
7.2 Energy Potentials of Molecular Hydrogen and Its Ions	187
References	201
Subject Index	211

Glossary of Terms

The fundamental constants used in atomic and molecular physics are listed in the table on the hardcover. Other fundamental physical constants are given in the report of the CODATA Task Group on Fundamental Constants, CODATA Bulletin No. 63, E.R. Cohen, B.N. Taylor: Rev. Mod. Phys. **59**, 1121 (1987). A list of symbols used in the book is also given in a Table.

List of Symbols

a, b, c	Inertial axes of molecule
A, B, C	Rotational constants
C_{σ}, C_{12}	Lennard-Jones interaction constants
C_n	$n = 6, 8$ and 10 van-der-Waals interaction constants
d_k	Degeneracy of the k -th vibration
D_e	Dissociative energy
f	Oscillator strength
I_a, I_b, I_c	Inertia molecular moments
J	Rotational quantum number
$K = A + 1$	Projection of the vibronic angular momentum onto the axis of symmetry
L	Electron orbital momentum
M_L	Projection of L onto the axis of symmetry
m	Electron mass
q	Franck-Condon factor
Q	Nuclear quadrupole moment
r_e	Equilibrium internuclear distance
R	Rotational momentum
S	Electron spin
v	Vibrational quantum number
α_c	Rotational-vibrational quantum number
σ	Bonding orbital; effective cross section
θ	Valence angle of molecule
Λ	Sum of M_L projections
ω	Frequency (wavenumber)