

Contents

II/20 Molecular Constants

Subvolume C: Non-linear Triatomic Molecules

Part 1: H₂O (HOH)

Part 6: HD¹⁶O (H¹⁶OD), HT¹⁶O (H¹⁶OT), HD¹⁷O (H¹⁷OD), HD¹⁸O (H¹⁸OD), DT¹⁶O (D¹⁶OT)

A	Introduction	IX
I	Energy level designations	IX
I.1	Vibrational assignment	IX
I.1.1	Normal and local modes	IX
I.1.2	Polyads	XI
I.1.3	Vibrational interactions	XV
I.2	Rotational assignment	XVI
I.3	Ortho–para transitions	XVII
I.4	MARVEL algorithm	XVII
II	Energy expressions referred to the ground state	XVII
II.1	Vibrational states	XVII
II.2	Simple expressions for the fundamental frequencies	XVII
III	Effective Hamiltonians	XVIII
III.1	<i>A</i> -reduced Watson-type rotational Hamiltonian	XVIII
III.2	Coudert Hamiltonian with Radau's coordinates	XX
III.3	Tyuterev Hamiltonian with Generating Function Model	XXI
III.4	Rotational Padé Hamiltonian operator	XXIII
III.5	Euler expansion of the Hamiltonian	XXV
IV	Perturbation-theory free Hamiltonians	XXVI
IV.1	Jensen Morse Oscillator–Rigid Bender Internal Dynamics Hamiltonian	XXVI
IV.2	Vibrational Hamiltonian expanded in terms of local Morse operators	XXVI
V	Potential energy	XXVI
V.1	Potential Energy Function (PEF) expanded as a power series	XXVI
V.2	Spectroscopically determined Potential Energy Surface (PES)	XXVII
V.2.1	Jensen's PES determined by variational calculation of rotation-vibration energies with MORBID Hamiltonian	XXVIII
V.2.2	Effective isotope-independent Born–Oppenheimer (B–O) PES with isotope-dependent adiabatic correction	XXVIII
V.2.3	Isotope-dependent PES from high-quality <i>ab-initio</i> analytical potential representation	XXIX
V.2.4	Semitheoretical PES by morphing <i>ab-initio</i> potential	XXX
V.2.5	Correction to the <i>ab-initio</i> PES expression from [2000Kai] for the determination of the barrier height	XXX
V.2.6	Force constants	XXX
VI	Dipole Moment Function (DMF)	XXXI
VI.1	One example of a Taylor series expansion form of the DMF	XXXI
VI.2	DMF expression in [97Cou]	XXXI
VI.3	Analytical expression of the Dipole Moment Surface in [97Par]	XXXII

VI.4	Dipole matrix elements in the DMS expansion used in [2005Tot2]	XXXII
VI.5	Transition moment for the bending-rotation Couderc Hamiltonian approach	XXXIII
VII	Intensities	XXXIV
VII.1	Line intensity	XXXIV
VII.2	Band intensity	XXXV
VII.3	Temperature dependence of the absorption	XXXVI
VII.4	Internal partition function	XXXVI
VIII	Line shape	XXXVII
VIII.1	Line profiles	XXXVII
VIII.1.1	Lorentz profile	XXXVII
VIII.1.2	Doppler profile	XXXVII
VIII.1.3	Voigt profile	XXXVII
VIII.2	Collision-broadening	XXXVIII
VIII.2.1	Self-broadening	XXXVIII
VIII.2.2	Foreign gas broadening	XXXVIII
VIII.2.3	Temperature dependence of the line broadening coefficients	XXXVIII
VIII.3	Family of H ₂ O lines	XXXVIII
IX	Conversion tables	XXXIX
IX.1	Conversion table for energy-related units and selected fundamental constants	XXXIX
IX.2	Intensity units and conversion table	XL
X	List of symbols	XLVI
XI	Survey	L
XI.1	Coupling constants	L
XI.2	Dipole moments	LI
XI.3	Dissociation energies	LI
XI.4	Force constants	LI
XI.5	Harmonic frequencies	LI
XI.6	Line positions with line intensity unit	LII
XI.7	Line positions with relative line intensities	LIII
XI.8	Line positions	LIV
XI.9	Line shape related parameters	LIV
XI.10	Partition function	LVI
XI.11	Potential	LVI
XI.12	Rovibrational energy levels	LVI
XI.13	Spectroscopic parameters	LVII
XI.14	Vibrational band intensities	LVIII
XI.15	Vibrational band origins	LIX
XII	Detailed survey of some tables	LX
B	Data	1
1	H ₂ O (HOH) cont.	1
1.9	HD ¹⁶ O (H ¹⁶ OD)	1
1.10	HT ¹⁶ O (H ¹⁶ OT)	289
1.11	HD ¹⁷ O (H ¹⁷ OD)	315
1.12	HD ¹⁸ O (H ¹⁸ OD)	332
1.13	DT ¹⁶ O (D ¹⁶ OT)	385
C	References	393