



# Contents

## Subvolume B1: Linear Triatomic Molecules $\text{BClH}^+$ ( $\text{HBCl}^+$ ) ... $\text{COSe}$ ( $\text{OCSe}$ )

<b>Introduction . . . . .</b>	<b>IX</b>
I      Energy level designations . . . . .	IX
II      Effective Hamiltonians . . . . .	X
II.1    Energy matrix . . . . .	X
II.1.1   Diagonal elements . . . . .	X
II.1.2   Off-diagonal elements . . . . .	XII
II.2    Energy expressions referred to the ground state . . . . .	XII
II.2.1   Vibrational states . . . . .	XIII
II.2.2   Rotational states . . . . .	XIII
II.3    Conversion table for energy-related units and selected fundamental constants . . . . .	XIV
III      Formulas for determining rotational constants . . . . .	XV
III.1    Effective parameters . . . . .	XV
III.2    Band center and band origin . . . . .	XVI
III.3    Comments on BHO (HBO) (see Chap. 6) . . . . .	XVII
III.4    Some specifics related to carbonyl sulfide, COS (OCS) (see Chap. 38) . . . . .	XVIII
III.4.1   Diagonalizing the energy matrix . . . . .	XVIII
III.4.2   Effective molecular parameters . . . . .	XVIII
III.4.3   Unperturbed vibrational states . . . . .	XIX
III.4.4   Effects of perturbations . . . . .	XIX
III.5    Quadrupole coupling . . . . .	XXI
IV      Potential energy function (PEF) . . . . .	XXI
IV.1    PEF expanded as a Taylor series . . . . .	XXI
IV.2    Curvilinear valence coordinates and Morse functions . . . . .	XXII
IV.3    Dimensionless normal coordinates . . . . .	XXII
IV.4    Specific forms of the PEF . . . . .	XXII
V      Dipole moment . . . . .	XXIV
V.1    General equations . . . . .	XXIV
V.2    Specifics related to COS (OCS) (see Chap. 38) . . . . .	XXV
VI      Intensities . . . . .	XXVII
VI.1    Intensities of spectral lines . . . . .	XXVII
VI.2    Integrated absorption intensities . . . . .	XXVII
VI.3    Total internal partition sum . . . . .	XXIX
VI.4 <i>F</i> -factors (Herman-Wallis factors) . . . . .	XXIX
VI.5    Intensity expressions . . . . .	XXX
VI.6    Intensity units and conversion table . . . . .	XXXI
VI.7    Line profiles . . . . .	XXXVIII
VI.7.1   Lorentz profile . . . . .	XXXVIII
VI.7.2   Doppler profile . . . . .	XXXVIII
VI.7.3   Voigt profile . . . . .	XXXVIII
VI.7.4   Galatry profile . . . . .	XXXIX

VI.8	Miscellaneous topics . . . . .	XXXIX			
VI.8.1	Some definitions related to collisions . . . . .	XXXIX			
VI.8.2	Foreign gas broadening . . . . .	XXXIX			
VI.8.3	Line coupling . . . . .	XL			
VI.8.4	Temperature dependence of broadening . . . . .	XL			
VI.9	Einstein coefficient of spontaneous emission . . . . .	XLI			
VI.10	Rotational state transfer . . . . .	XLI			
VII	Renner-Teller effect (some aspects) . . . . .	XLII			
VIII	List of symbols . . . . .	XLIV			
<b>Data</b>	. . . . .	1			
1	BClH <sup>+</sup> (HBCl <sup>+</sup> ) . . . . .	1	21	CFN (FCN) . . . . .	59
2	BClH <sup>+</sup> (BClH <sup>+</sup> ) . . . . .	9	22	CFN (FNC) . . . . .	76
3	BCIO (OBCl) . . . . .	10	23	CFP (FCP) . . . . .	78
4	BFH <sup>+</sup> (HBF <sup>+</sup> ) . . . . .	13	24	CHN (HCN) . . . . .	79
5	BFO (FBO) . . . . .	16	25	CHN (HNC) . . . . .	183
6	BHO (HBO) . . . . .	17	26	CHO <sup>+</sup> (HCO <sup>+</sup> ) . . . . .	198
7	BHS (HBS) . . . . .	26	27	CHO <sup>+</sup> (HOC <sup>+</sup> ) . . . . .	202
8	BO <sub>2</sub> (OBO) . . . . .	34	28	CHP (HCP) . . . . .	206
9	BeF <sub>2</sub> (FBeF) . . . . .	38	29	CHS <sup>+</sup> (HCS <sup>+</sup> ) . . . . .	212
10	CBaN (BaCN) . . . . .	39	30	CIN (ICN) . . . . .	216
11	CBaN (BaNC) . . . . .	40	31	CLiN (LiCN) . . . . .	222
12	CBeN (BeCN) . . . . .	40	32	CLiN (LiNC) . . . . .	224
13	CBeN (BeNC) . . . . .	40	33	CMgN (MgCN) . . . . .	226
14	CBrN (BrCN) . . . . .	40	34	CMgN (MgNC) . . . . .	227
15	CBrN <sup>+</sup> (BrCN <sup>+</sup> ) . . . . .	43	35	CNO <sup>-</sup> (NCO <sup>-</sup> ) . . . . .	230
16	CCaN (CaCN) . . . . .	46	36	CNS (NCS) . . . . .	231
17	CCaN (CaNC) . . . . .	46	37	CNS <sup>-</sup> (NCS <sup>-</sup> ) . . . . .	233
18	CClN (ClCN) . . . . .	46	38	COS (OCS) . . . . .	238
19	CClN <sup>+</sup> (ClCN <sup>+</sup> ) . . . . .	51	39	COSe (OCSe) . . . . .	416
20	CClP (ClCP) . . . . .	52			
<b>References</b>	. . . . .				447

