

Volume II/20: Molecular Constants Mostly from Infrared Spectroscopy

Editor: G. Guelachvili

Subvolume b2 α : Linear Triatomic Molecules: CO₂(OCO)

Authors: G. Guelachvili, K. Narahari Rao

1997. LXI, 415 pages. ISBN 3-540-58852-3

Contents

Introduction

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 of subvolume II/20b1)	XVII
III.4	Some specifics related to COS (OCS) (see Chap. 38 of subvolume II/20b1)	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. 3 8 of subvolume II/20b1)	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	Some functional relations specially applicable to the molecular constants of CO ₂	XLIV
VIII.1	Designations of the energy levels of CO ₂	XLIV
VIII.2	Resonances in CO ₂	XLIV
VIII.3.1	Potential-energy function (PEF)	XLVIII
VIII.3.2	Interaction potential	XLVIII
VIII.4.1	Dipole moment	XLVIII
VIII.4.2	Transition dipole moment	XLIX
VIII.5	HITELOR (High Temperature Low Resolution data base)	XLIX
VIII.6	Line mixing	XLIX
VIII.7	Several functional relations in which effects of collisions are included	LI
VIII.7.1	Collisional broadening	LI
VIII.7.2	Binary absorption coefficient	LI
VIII.7.3	Normalized absorption coefficient	LI
VIII.7.4	Collision induced contribution in the band intensity	LII
VIII.8	Self broadening and its temperature dependence	LII
VIII.9	Foreign gas broadening	LII
VIII.10	Transmittance at the center of a spectral line	LII
VIII.11	Line mixing (temperature and pressure dependence)	LIII
VIII.11.1	Temperature dependence of line mixing	LIII
VIII.11.2	Pressure dependence of line mixing	LIII
VIII.12	Some formulas for the absorption coefficient $k(\nu)$	LIII
VIII.12.1	Impact approximation	LIII
VIII.12.2	First order theory of Rosenkranz	LIV
VIII.13	CO ₂ laser wave guide amplification and power saturation	LIV
IX	List of symbols	LVI
1	BCIH⁺ (HBCI⁺) ... 39 COSe (OCSe)	see subvolume II/20b1
40	COO (OCO)	1
40.1	¹²C¹⁶O¹⁶O (¹⁶O¹²C¹⁶O)	1
Survey	1	
Arrangement of the tables		1
Data	79	
40.2 ... 40.14	¹²C¹⁶O¹⁷O (¹⁶O¹²C¹⁷O) ... ¹⁴C¹⁸O¹⁸O (¹⁸O¹⁴C¹⁸O)	see subvolume II/20b2β
References		391