

# Content

## II/20 Molecular Constants

### Subvolume B4: Linear Triatomic Molecules

$\text{COO}^+$  ( $\text{OCO}^+$ ),  $\text{CFeO}$  ( $\text{FeCO}$ ),  $\text{CFeO}^-$  ( $\text{FeCO}^-$ ),  $\text{CNN}$  ( $\text{NCN}$ ),  
 $\text{CNO}$  ( $\text{NCO}$ ),  $\text{CNO}$  ( $\text{CNO}$ ),  $\text{CNO}$  ( $\text{CON}$ ),  $\text{CNO}^-$  ( $\text{NCO}^-$ )

### Introduction ..... IX

(Specific comments related to some of the molecules considered in Chaps. 1...39 of subvolume II/20B1, in Chaps. 40.1 ... 40.14 and in Chaps. 41.1 ... 41.12 are retained in the present introduction due to their possible general applicability)

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. 38 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	F-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 <sub>2</sub> . . . . .	XLIV
VIII.1	Designations of the energy levels of CO <sub>2</sub> . . . . .	XLIV
VIII.2	Resonances in CO <sub>2</sub> . . . . .	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 $k(n)$ . . . . .	LIII
VIII.12.1	Impact approximation. . . . .	LIII
VIII.12.2	First order theory of Rosenkranz . . . . .	LIV
VIII.13	CO <sub>2</sub> laser wave guide amplification and power saturation . . . . .	LIV
IX	Some symbolism appearing in N <sub>2</sub> O data . . . . .	LV
X	Some symbolism appearing in CO <sub>2</sub> <sup>+</sup> , CFeO, CFeO <sup>-</sup> , CNN, CNO and CNO <sup>-</sup> data . . . . .	LVIII
X.1	Aspects of some notations in polyatomic molecules. . . . .	LVIII
X.2	CO <sub>2</sub> <sup>+</sup> . . . . .	LVIII
X.3	CFeO for which the electronic ground state is $^3\Sigma^-$ . . . . .	LXIII
X.4	CNN (NCN) . . . . .	LXIII
XI	List of symbols . . . . .	LXVI

**Data**

1	BClH <sup>+</sup> (HBCl <sup>+</sup> ) ... 39	COSe (OCSe) . . . . .	see subvolume II/20B1
40.1	<sup>12</sup> C <sup>16</sup> O <sup>16</sup> O ( <sup>16</sup> O <sup>12</sup> C <sup>16</sup> O)	... . . . .	see subvolume II/20B2α
40.2 ... 40.14	<sup>12</sup> C <sup>16</sup> O <sup>17</sup> O ( <sup>16</sup> O <sup>12</sup> C <sup>17</sup> O) ... <sup>14</sup> C <sup>18</sup> O <sup>18</sup> O ( <sup>18</sup> O <sup>14</sup> C <sup>18</sup> O).	. . . . .	see subvolume II/20B2β
41.1 ... 41.12	<sup>14</sup> N <sup>14</sup> N <sup>16</sup> O ( <sup>14</sup> N <sup>14</sup> N <sup>16</sup> O) ... <sup>15</sup> N <sup>15</sup> N <sup>18</sup> O ( <sup>15</sup> N <sup>15</sup> N <sup>18</sup> O).	. . . . .	see subvolume II/20B3
<b>42</b>	<b>COO<sup>+</sup> (OCO<sup>+</sup>) ... 50</b>	<b>CNO<sup>-</sup> (NCO<sup>-</sup>) (survey)</b> . . . . .	<b>1</b>
<b>References</b> . . . . .			
168			

# **Survey of Content**

## **II/20 Molecular Constants**

### **Subvolume B4: Linear Triatomic Molecules**

$\text{COO}^+$  ( $\text{OCO}^+$ ),  $\text{CFeO}$  ( $\text{FeCO}$ ),  $\text{CFeO}^-$  ( $\text{FeCO}^-$ ),  $\text{CNN}$  ( $\text{NCN}$ ),  
 $\text{CNO}$  ( $\text{NCO}$ ),  $\text{CNO}$  ( $\text{CNO}$ ),  $\text{CNO}$  ( $\text{CON}$ ),  $\text{CNO}^-$  ( $\text{NCO}^-$ )

**Introduction**

**List of symbols**

**Table**

**References**