

Contents

	Page		Page
1. Introduction	1	h. $v=7$	24
2. Electronic structure of CO and CO ⁺	2	i. $v=8$	25
2.1 Electronic structure	2	j. $v=9$	25
2.2 Numerical calculations	4	k. $v=10$	25
a. Semiempirical	4	l. $v=11$	25
b. Single configuration	4	m. $v=12$	25
c. Configuration interaction	4	n. $v=13$	25
2.3 Rydberg states and Rydberg series	5	4.2 E ¹ Π state	25
3. Electronic spectrum of CO and CO ⁺	5	4.3 a ³ Π state	25
3.1 A ¹ Π—X ¹ Σ ⁺ Fourth Positive system (2800–1140 Å) R	6	4.4 d ³ Δ _i state	26
3.2 B ¹ Σ ⁺ —A ¹ Π Ångstrom system (6620–4120 Å) V	8	4.5 f ³ Σ ⁺ state	26
3.3 C ¹ Σ ⁺ —A ¹ Π Herzberg system (5710–3680 Å) V	9	4.6 b ³ Σ ⁺ state	26
3.4 Hopfield-Birge systems (1810–950 Å)	10	4.7 A ² Π _i state of CO ⁺	26
a. B ¹ Σ ⁺ , C ¹ Σ ⁺ , E ¹ Π, F(¹ Σ ⁺), G(¹ Π), and b ³ Σ ⁺ —X ¹ Σ ⁺	10	a. $v=5$	26
b. a ³ Σ ⁺ —X ¹ Σ ⁺ (1810–1280 Å) R	10	b. $v=10$	27
3.5 a ³ Π—X ¹ Σ ⁺ Cameron system (5800–1770 Å) R	11	5. Dissociation energies, predissociations, and convergence limits	27
3.6 b ³ Σ ⁺ —a ³ Π Third Positive system (3820–2660 Å) V	12	5.1 Dissociation energy of CO	27
3.7 c ³ Σ ⁺ —a ³ Π 3A system (2710–2300 Å) V	13	5.2 Predissociations and convergence limits	28
3.8 a ³ Σ ⁺ —a ³ Π Asundi system (8590–3900 Å) R	14	a. Predissociation of the B ¹ Σ ⁺ state	28
3.9 d ³ Δ _i —a ³ Π Triplet system (7500–3770 Å) R	15	b. Predissociation of the b ³ Σ ⁺ state	28
3.10 e ³ Σ ⁻ —X ¹ Σ ⁺ transition (1540–1240 Å) R	16	c. Predissociation of the C ¹ Σ ⁺ state	29
3.11 C ¹ Σ ⁺ —a ³ Σ ⁺ Knauss system (3250–2930 Å) V	17	d. Suspected predissociation of the e ³ Σ ⁺ state	29
3.12 Kaplan bands (2750–2520 Å)	17	e. Convergence limit of the a ³ Σ ⁺ state	29
3.13 d ³ Δ _i —X ¹ Σ ⁺ transition (1620–1230 Å) R	17	f. Convergence limit of the F(¹ Σ ⁺) state	30
3.14 e ³ Σ ⁻ —a ³ Π Herman system (5430–4270 Å) R	17	5.3 Dissociation energy of CO ⁺ , ionization potentials and Rydberg series	30
3.15 E ₀ ¹ Σ ⁺ —X ¹ Σ ⁺ , ¹ Π—X ¹ Σ ⁺ , and several unidentified transitions in the vacuum UV region (1180–930 Å)	17	5.4 Dissociation energy of CO ²⁺	31
3.16 f ³ Σ ⁺ —a ³ Π transition (2980–2670 Å) R	18	6. The vibration-rotation spectrum of CO	31
3.17 I ¹ Σ ⁻ —X ¹ Σ ⁺ transition (1520–1460 Å) R	18	6.1 Δ <i>v</i> =1 sequence	31
3.18 Unidentified bands	19	6.2 Overtone sequence and other overtone bands	31
3.19 P, Q, R, S, T—X ¹ Σ ⁺ Tanaka systems (800–630 Å) R	19	7. Rotational spectrum of CO (microwave and far infrared)	32
3.20 Rydberg series (940–630 Å)	19	7.1 Rotational transitions in CO	32
3.21 B ² Σ ⁺ —X ² Σ ⁺ First Negative system of CO ⁺ (3150–1800 Å) R	20	7.2 Stark effect	32
3.22 A ² Π _i —X ² Σ ⁺ Comet Tail system of CO ⁺ (7200–3080 Å) R	21	7.3 Zeeman effect	32
3.23 B ² Σ ⁺ —A ² Π _i Baldet-Johnson intercombination system of CO ⁺ (4240–3310 Å) V	22	7.4 Quadrupole hyperfine structure	33
4. Perturbations	22	8. Raman, Stark, and Zeeman effects in electronic spectra of CO and CO ⁺	33
4.1 A ¹ Π state	22	8.1 Raman effect	33
a. $v=0$	22	8.2 Stark effect	33
b. $v=1$	23	8.3 Zeeman effect	33
c. $v=2$	24	9. Molecular energy levels and potential energy curves	34
d. $v=3$	24	10. Transition probabilities and lifetimes (electronic spectra)	35
e. $v=4$	24	10.1 A ¹ Π—X ¹ Σ ⁺ Fourth Positive system	35
f. $v=5$	24	10.2 B ¹ Σ ⁺ —A ¹ Π Ångstrom system	35
g. $v=6$	24	10.3 C ¹ Σ ⁺ —A ¹ Π Herzberg system	35
		10.4 b ³ Σ ⁺ —a ³ Π Third Positive system	35
		10.5 a ³ Σ ⁺ —a ³ Π Asundi system	36
		10.6 a ³ Π—X ¹ Σ ⁺ Cameron system	36
		10.7 b ³ Σ ⁺ —X ¹ Σ ⁺ Hopfield-Birge system	36
		10.8 a ³ Σ ⁺ —X ¹ Σ ⁺ Hopfield-Birge system	36
		10.9 d ³ Δ _i —a ³ Π Triplet system	36
		10.10 A ² Π _i —X ² Σ ⁺ (CO ⁺) Comet Tail system	36
		10.11 B ² Σ ⁺ —X ² Σ ⁺ (CO ⁺) First Negative system	37

Contents—Continued

	Page		Page
10.12 $B^2\Sigma^+ - A^2\Pi_i$ (CO^+) Baldet-Johnson system.....	37	12. Tables and figures.....	38a
10.13 Ionization of CO	37	13. References.....	78
10.14 Miscellaneous.....	37	Appendix A—notation and terminology.....	85
11. Summary and conclusion.....	37	Appendix B—physical constants and conversion factors.....	87

Tables

1. Molecular constants, electron configurations, and dissociation products for the electronic states of CO and CO^+ . Supplement: Rydberg states.....	38a	20. Band heads of the Kaplan system (R).....	50
2. Electron configurations for states of CO and CO^+	39	21. Band heads of the $d^3\Delta_i \leftarrow X^1\Sigma^+$ system (R).....	51
3. Band heads of the $A^1\Pi - X^1\Sigma^+$ Fourth Positive system (R).....	40	22. Band heads of the $e^3\Sigma^- \rightarrow a^3\Pi$ Herman system (R).....	51
(a) Emission.....	40	23. Band heads of the $E_0^1\Sigma^+ \rightarrow X^1\Sigma^+$ system (R).....	51
(b) Absorption.....	41	24. Band heads of the $^1\Pi \rightarrow X^1\Sigma^+$ system (R).....	51
4. Deslandres table for the band origins of the $A^1\Pi - X^1\Sigma^+$ Fourth Positive system.....	42	25. Band heads of the $f^3\Sigma^+ \rightarrow a^3\Pi$ system (R).....	51
5. Band heads and origins of the $A^1\Pi - X^1\Sigma^+$ Fourth Positive system of $C^{13}O^{16}$ (R).....	43	26. Band heads of the Tanaka systems (absorption).....	52
(a) Emission.....	43	(a) $P \leftarrow X^1\Sigma^+$	52
(b) Absorption.....	43	(b) $Q \leftarrow X^1\Sigma^+$	52
6. Band heads and origins of the $B^1\Sigma^+ \rightarrow A^1\Pi$ Ångström system (V).....	43	(c) $R \leftarrow X^1\Sigma^+$	52
7. Band heads and origins of the $B^1\Sigma^+ \rightarrow A^1\Pi$ system of $C^{13}O^{16}$ (V).....	43	(d) $S \leftarrow X^1\Sigma^+$	52
8. Band heads and origins of the $C^1\Sigma^+ \rightarrow A^1\Pi$ Herzberg system (V).....	43	(e) $T \leftarrow X^1\Sigma^+$	52
9. Band heads of the Hopfield-Birge systems.....	44	27. $B^2\Sigma^+(CO^+) \leftarrow X^1\Sigma^+$ “ β ” Rydberg series.....	52
(a) $B^1\Sigma^+ \leftrightarrow X^1\Sigma^+$	44	28. $A^2\Pi_i(CO^+) \leftarrow X^1\Sigma^+$ “ α ” Rydberg series.....	53
(b) $C^1\Sigma^+ \leftrightarrow X^1\Sigma^+$	44	29. $X^2\Sigma^+(CO^+) \leftarrow X^1\Sigma^+$ Rydberg series.....	53
(c) $E^1\Pi \leftrightarrow X^1\Sigma^+$	44	30. Band heads of the $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ First Negative system of CO^+ (R).....	53
(d) $F(^1\Sigma^+) \leftarrow X^1\Sigma^+$	44	31. Band origins of the $B^2\Sigma^+ - X^2\Sigma^+$ First Negative system of CO^+	54
(e) $G(^1\Pi) \leftarrow X^1\Sigma^+$	44	32. Band heads of the $A^2\Pi_i \rightarrow X^2\Sigma^+$ Comet Tail system of CO^+ (R).....	54
(f) $b^3\Sigma^+ \leftrightarrow X^1\Sigma^+$	44	33. Band origins of the $A^2\Pi_i - X^2\Sigma^+$ Comet Tail system of CO^+	55
10. Band heads and origins of the $a^3\Sigma^+ \leftarrow X^1\Sigma^+$ Hopfield-Birge system (R).....	44	34. Band heads of the $B^2\Sigma^+ \rightarrow A^2\Pi_i$ Baldet-Johnson system of CO^+ (V).....	55
11. Band heads of the $a^3\Pi - X^1\Sigma^+$ Cameron system (R).....	45	35. Miscellaneous unclassified bands.....	55
(a) Emission.....	45	(a) Band heads observed together with the $A^1\Pi - X^1\Sigma^+$ Fourth Positive system (Emission).....	55
(b) Absorption.....	45	(b) Band heads observed in absorption.....	55
12. Band origins of the $a^3\Pi - X^1\Sigma^+$ Cameron system.....	45	(c) Band heads observed with the $a^3\Sigma^+ \rightarrow a^3\Pi$ Asundi system.....	56
13. Band heads of the $b^3\Sigma^+ \rightarrow a^3\Pi$ Third Positive system (V).....	46	(d) Band heads observed in emission by Tschulanovsky and Gassilevitch.....	56
14. Band heads of the $c^3\Sigma^+ \rightarrow a^3\Pi$ 3A system (V).....	46	(e) Triplet bands observed in emission.....	56
15. Band heads of the $a^3\Sigma^+ \rightarrow a^3\Pi$ Asundi system (R).....	47	(f) Unclassified absorption maxima.....	56
16. Band heads of the $d^3\Delta_i \rightarrow a^3\Pi$ Triplet system (R).....	49	(g) Unclassified absorption bands.....	57
(a) Identified bands.....	49	(h) Emission and absorption bands of Anand.....	57
(b) Unassigned bands.....	50	(i) Band heads observed together with the $A^2\Pi_i \rightarrow X^2\Sigma^+$ Comet Tail system of CO^+	57
17. Band origins of the $d^3\Delta_i - a^3\Pi$ Triplet system.....	50	(j) Band heads observed with the $B^2\Sigma^+ \rightarrow A^2\Pi_i$ system of CO^+	57
18. Band heads and origins of the $e^3\Sigma^- \leftarrow X^1\Sigma^+$ system (R).....	50	36. Rotational constants for the $X^1\Sigma^+$ state.....	58
19. Band heads of the $C^1\Sigma^+ \rightarrow a^3\Sigma^+$ Knauss system (V).....	50	37. Rotational constants for the $A^1\Pi$ state.....	58
		38. Rotational constants for the $B^1\Sigma^+$ state.....	58

Tables—Continued

	Page		Page
39. Rotational constants for the $C^1\Sigma^+$ state.....	58	centroids, and I_∞ for the $B^1\Sigma^+-A^1\Pi$ Ångstrom system.....	66
40. Rotational constants for the $E^1\Pi$ state.....	59	62. Franck-Condon factors for the $C^1\Sigma^+-A^1\Pi$ Herzberg system.....	66
41. Rotational constants for the $a^3\Sigma^+$ state.....	59	63. Franck-Condon factors, band strengths, r -centroids, and I_∞ for the $b^3\Sigma^+-a^3\Pi$ Third Positive system.....	66
42. Rotational constants for the $a^3\Pi$ state.....	59	64. Franck-Condon factors for the $a^3\Sigma^+-a^3\Pi$ Asundi system.....	66
43. Rotational constants for the $b^3\Sigma^+$ state.....	59	65. Franck-Condon factors for the $a^3\Pi-X^1\Sigma^+$ Cameron system.....	67
44. Rotational constants for the $c^3\Sigma^+$ state.....	59	66. Franck-Condon factors for the $b^3\Sigma^+-X^1\Sigma^+$ Hopfield-Birge system.....	67
45. Rotational constants for the $d^3\Delta_i$ state.....	59	67. Franck-Condon factors for the $a^3\Sigma^+-X^1\Sigma^+$ Hopfield-Birge system.....	67
46. Rotational constants for the $e^3\Sigma^-$ state.....	59	68. Franck-Condon factors, r -centroids, and I_∞ for the $d^3\Delta_i-a^3\Pi$ Triplet system.....	68
47. Rotational constants for the $E_0^1\Sigma^+$ state.....	59	69. (a) Franck-Condon factors, r -centroids, and wavelengths for the $A^2\Pi_i-X^2\Sigma^+$ Comet Tail system of CO^+	69
48. Rotational constants for the $^1\Pi$ state.....	59	(b) Smoothed band strengths and I_∞ for the $A^2\Pi_i-X^2\Sigma^+$ Comet Tail system of CO^+	70
49. Rotational constants for the $f^3\Sigma^+$ state.....	59	70. Franck-Condon factors, r -centroids, and wavelengths for the $B^2\Sigma^+-X^2\Sigma^+$ First Negative system of CO^+	71
50. Rotational constants for the $X^2\Sigma^+$ state of CO^+	60	71. Franck-Condon factors, r -centroids, and wavelengths for the $B^2\Sigma^+-A^2\Pi_i$ Baldet-Johnson system of CO^+	72
51. Rotational constants for the $A^2\Pi_i$ state of CO^+	60	72. Franck-Condon factors for ionizing transitions.....	73
52. Rotational constants for the $B^2\Sigma^+$ state of CO^+	60	73. (a) Lifetimes, Einstein coefficients, and oscillator strengths.....	74
53. Doublet splitting constants for states of CO^+	60	(b) Einstein coefficients, absolute band strengths, and band oscillator strengths for the $A^2\Pi_i-X^2\Sigma^+$ Comet Tail system of CO^+	74
54. Perturbations of the electronic states of CO and CO^+	60	(c) Absolute f -values for the $A^1\Pi-X^1\Sigma^+$ Fourth Positive system.....	74
(a) $A^1\Pi$ state.....	60	74. Potential energy of the electronic states of CO and CO^+	75
(b) $E^1\Pi$ state.....	62		
(c) $a^3\Pi$ state.....	62		
(d) $d^3\Delta_i$ state.....	62		
(e) $f^3\Sigma^+$ state.....	62		
(f) $b^3\Sigma^+$ state.....	62		
(g) $A^2\Pi_i$ state of CO^+	63		
55. Observed predissociations in $C^{12}O^{16}$ and $C^{13}O^{16}$	63		
56. Vibration-rotation bands of CO in the infrared region.....	64		
57. Dipole moments for states of CO and CO^+	64		
58. Rotational frequencies, rotational constants, and magnetic moments of carbon monoxide.....	64		
59. Hyperfine structure.....	65		
60. (a) Franck-Condon factors for the $A^1\Pi-X^1\Sigma^+$ Fourth Positive system.....	65		
(b) r -centroids (Å) for the $A^1\Pi-X^1\Sigma^+$ Fourth Positive system.....	65		
61. Franck-Condon factors, band strengths, r -			

Figures

1. Potential energy curves for CO and CO^+	77	2. Energy level diagram for CO and CO^+	77
--	----	---	----

