Appendix A
List of Symbols

For convenience, many symbols frequently used in the text are listed below alphabetically. Some of the symbols may play a dual role, in which case the meaning should be obvious from the context. A number in parentheses refers to an Eq. number (or the text or footnote near that Eq. number) in which the symbol is defined or appears for the first time; in a few cases a page number, Table number, Sect. number, footnote (fn.) number, or Fig. number is given instead. Quantum number is abbreviated as q. n.

Quantum numbers (atomic):

Symbol	Description	Eq. No.
$j = l \pm s$	Inner q. n. of an electron	(3.13)
$J = L + S$	Inner (total angular momentum) q. n. of a state	(5.51b)
l	Azimuthal (orbital) q. n. of an electron	(3.1) and (3.2)
$L = \sum l$	Azimuthal (orbital) q. n. of a state	(5.51c)
m_l	Magnetic orbital q. n. of an electron	(3.1)
m_s	Magnetic spin q. n. of an electron	(3.1)
M	Total magnetic q. n.	(5.51d)
n	Principal q. n. of an electron	(3.1)
s	Spin q. n. of an electron	(3.13)
$S = \sum s$	Spin q. n. of a state	(5.51e)
κ	Relativistic azimuthal q. n. of an electron	(3.15a) and (3.15b)
μ	Relativistic magnetic q. n. of an electron	(3.18a) and (3.18b)

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402,
DOI 10.1007/978-1-4614-8797-5, © Springer Science+Business Media New York 2014

Quantum numbers (molecular)[1]:

Symbol	Description	Eq. No.
I	Nuclear spin q. n.	p. 62
J	Rotational q. n.	(3.63)
K	Total angular momentum q. n. apart from spin	(3.80)
L	Electronic orbital angular momentum q. n.	p. 61
S	Electron spin angular momentum q. n.	pp. 59–62
v	Vibrational q. n.	(3.62)
Λ	q. n. projection of L on internuclear axis	pp. 59–62
Σ	q. n. for projection of S on internuclear axis	pp. 59–62
$\Omega = \Lambda + \Sigma$	Total angular momentum q. n. about internuclear axis	p. 59

General list of symbols:

Symbol	Description	Eq. No.
A	Atomic mass	
A	Conversion coefficient for extinction, absorption, and scattering	(2.56)
A_i	IR molar absorption lengths	(5.116)
$A_i(r)$	Exchange Coulomb interaction	(3.3) and (3.4a)
A_v	Rotational constant for vibrational level (for diatomics the subscript v can be deleted)	p. 61 and (3.94)
A_ul	Radiation Einstein coefficient	(5.56a) and (5.57a)
$\boldsymbol{A}$	Vector potential for electromagnetic field	(5.48)
$\mathcal{A}$	Spin coupling constant for a multiplet	(3.78)
$\mathcal{A}_\nu$	Albedo at frequency ν	(2.8)
a_o	Radius of first Bohr orbit of hydrogen	p. 30
a_l^s	Scattering coefficient	(5.267a) and (5.269b)
$\hat{a}_i$	Activity of chemical species i	(4.74) and (4.76)
$a_\mathrm{S} = 4\sigma/c$	Stefan's radiation energy density constant	(2.48)
$B(T)$	Planck radiance at temperature T	(2.36)
B_e	Rotational constant for equilibrium position	(3.64b)
$B_{ij}(r)$	Exchange Coulomb interaction	(3.3) and (3.4b)
B_ul	Radiation Einstein coefficient for radiation energy density	(5.56a) and (5.57b)
B_v	Rotational constant for vibrational level	(3.64a) and (3.94)
$B_\nu(T)$	Planck photon frequency distribution function at frequency ν and temperature T	(2.4)

[1] Herzberg (1950, Chap. V) includes helpful vector diagrams illustrating various cases of coupling of electronic and rotational motions.

$\boldsymbol{B}$	Magnetic induction	(5.2)
b_l^{s}	Scattering coefficient	(5.267b) and (5.269b)
b	Ray's asymmetry parameter	(3.94)
C_{ij}	Collisional rate between states i and j	(2.1)
C_{v}	Rotational constant for vibrational level	(3.94)
c	Speed of light	
$c^{(k)}$	Gaunt angular coefficient	(3.8) and (3.9)
c_{ik}	Radiation scattering tensor	(5.210)
$D(\rho, T)$	Photon diffusion coefficient at density ρ and temperature T	(2.49)
$D^{\mathrm{a}}(u)$	Reduced absorption coefficient without stimulated emission	(2.55b)
$D^{\mathrm{a}'}(u)$	Reduced absorption coefficient with stimulated emission	(2.55a)
D_e	Width of Gauss distribution at e^{-1} of maximum	(7.15a)
$D^{\mathrm{s}}(u)$	Reduced scattering coefficient	(6.60)
$D^{\mathcal{T}}(u)$	Reduced transport extinction coefficient	(2.55a) and (2.55b)
$D^{\mathrm{s}\mathcal{T}}(u)$	Reduced transport scattering coefficient	(2.55a)
D_n	Binding energy of molecule	(3.65)
$\boldsymbol{D}$	Electric displacement	(5.1)
$\mathbf{D}(\theta, \phi, \chi)$	Dyad relating space-fixed axes to molecule-fixed axes in terms of Eulerian angles	(5.99)
d_i	Spin–orbit angular interaction of an electron	(3.12)
E	Total energy of molecule, atom, or ion	(3.59) and (4.1)
E_{o}	Continuum lowering energy	(4.2) and (4.6)
E_{f}	Interaction energy with free electrons	(4.1)
E_i	Binding energy of an electron in level i	(3.3), (3.15a), and (3.15b)
$\overline{E_i}$	Mean binding energy of electron in level i	(3.47)
$E_i^{(\mathrm{n})}$	Binding energy of level i in neutral atom	(3.47)
E_{ij}	Electron–electron interaction energy	(3.46)
$E_{ij}^{(\mathrm{i})}$	Electron–electron interaction energy in an ion	(3.48)
$E_{ij}^{(\mathrm{n})}$	Electron–electron interaction energy in a neutral atom	(3.50)
E_J	Rotational energy in a molecule	(3.61a)
E_{kin}	Mean kinetic energy of ion and electrons	(4.34)
E_n	Electronic energy in a molecule	(3.61a)
E_{pot}	Mean potential energy	(4.33)
E_{v}	Vibrational energy in molecule	(3.61a)
$E_{\mathrm{v}J}$	Sum of vibrational and rotational energy in molecule	(3.67)
$\boldsymbol{E}$	Electric field	(5.2)
$\lvert\boldsymbol{E}_{\mathrm{o}}\rvert$	Magnitude of electric field vector $\boldsymbol{E}_{\mathrm{o}}$ (in contrast to continuum lowering energy; see E_{o})	(5.260a)
$\mathcal{E}_{\mathrm{I}i}$	Energy of excitation above ground state of ionization stage I	(4.59) and (4.60)
$\mathcal{E}_{\mathrm{v}}$	Vibrational energy eigenvalue	p. 161 fn. 21
e	Charge of electron	
$\mathrm{erf}(x)$	Error function	(6.4)

(continued)

(continued)

Symbol	Description	Eq. No.
$\boldsymbol{e}_\nu$	Polarization vector	(5.55)
F	Helmholtz free energy	(4.21)
$F^+(\rho, T)$	Total outflowing flux density (exitance) at density ρ and temperature T	(2.34)
$F^-(\rho, T)$	Total inflowing flux density (irrandiance) at density ρ and temperature T [in contrast see $F^+(\rho, T)$]	
$F^{(k)}$	Slater integral	(3.8b)
$F_i(r)$	r times the small Dirac wave function	(3.15a)
F_J	Rotational term value in molecule	(3.61b)
F_ν^+	Outflowing component of flux (exitance) at frequency ν	(2.14)
F_ν^-	Inflowing component of flux (irradiance) at frequency ν	(2.15)
$F(\boldsymbol{k})$	Form factor	(5.204)
$F_{\mathrm{coh}}(\nu)$	Coherent form factor	(5.214)
$F_{\mathrm{inc}}(\nu)$	Incoherent form factor	(5.216)
$\boldsymbol{F}(\boldsymbol{r})$	Conductive heat flow	(9.1a)
$\boldsymbol{F}$	Total flux	(2.46)
$\boldsymbol{F}_\nu$	Net flux at frequency ν	(2.13)
$f(\eta, \delta)$	Correction factor for electron correlation	(6.51)
$f(v)dv$	Maxwell velocity distribution function	(6.14)
$f_{\mathrm{e}}(\boldsymbol{x}, \boldsymbol{p})$	Electron distribution function	(9.17)
$f_{\mathrm{i}}(\boldsymbol{x}, \boldsymbol{p})$	Ion distribution function	(9.22)
f_{lu}	Oscillator strength	(5.59)
f_{S}	Surface geometry coefficient	(2.30)
G	Gibbs free energy	(4.67)
$G_i(r)$	r times the large Dirac wave function	(3.15b)
$G^{(k)}$	Slater integral	(3.8)
G_{v}	Vibrational term value in molecule	(3.61b)
$G^{LS}_{L_i S_i}$	Racah fractional parentage coefficient	(5.85b)
$\mathcal{G}(\nu)$	Spectral function of a binary complex of a supermolecular transition in a rarefied gas, such as $\mathrm{v}_1 j_1 \mathrm{v}_2 j_2 \rightarrow \mathrm{v}_1' j_1' \mathrm{v}_2' j_2'$, thermodynamically averaged at a given temperature [identical to $\breve{g}(\nu; T)\, for$ atom–atom pairs].	(8.32) and (8.33)
g	Bispinor	(3.19)
g_{i}	Statistical weight of state or level i	(2.2) and (5.61)
$g_{\mathrm{bf},i}$	Bound–free Gaunt factor for an electron in level i	(5.86)
g_{ff}	Free–free Gaunt factor	(5.95) and (5.97)
$\breve{g}(\nu; T)$	Spectral function [weighted sum of $\mathcal{G}(\nu)$]	(8.32)
$\breve{g}(\nu; \mathrm{v}\mathrm{v}', T)$	Spectral function [see also $\phi(\nu)$]	(8.39)
H	Enthalpy	(4.67)
H	Total Hamiltonian ($H = H_0 + H'$)	(5.163) and (5.179)
H_0	Hamiltonian without radiation interaction	(5.150)
H'	Hamiltonian for radiation interaction	(5.46) and (5.48)

H_J	Hamiltonian for rotation	(3.77)
H_{nv}	Hamiltonian for electronic vibration	(3.77)
$H(\beta)$	Holtsmark distribution	(7.72)
$H_n(x)$	Hermite polynomial	(5.131), Appendix C
$\boldsymbol{H}$	Magnetic field	(5.4)
$\mathcal{H}$	Voigt function	(7.18)
$\mathcal{H}'$	Total Hamiltonian (including higher order terms)	(5.45)
h	Planck constant	
$h_l^{(1)}(x)$	Spherical Hankel functions of the first kind	(5.266), Appendix C p. 250 fn. 73
$h_l^{(2)}(x)$	Spherical Hankel functions of the second kind	(5.266), Appendix C p. 250 fn. 73
I	Irradiance (radiative flux), magnitude of Poynting vector	(5.35a)
I_A	Moment of inertia about the A axis (for diatamics it is the moment of inertia of the electrons about the internuclear axis)	p. 61
$I_k(\eta)$	Fermi integral of order k	(4.13)
I_ν	Spectral radiance at frequency ν	(2.3)
$\mathcal{I}$	Action	(3.67)
J	Total zeroth angular moment of radiance	(2.52)
J_ν	Zeroth angular moment of spectral radiance at frequency ν	(2.18)
$\boldsymbol{J}_e$	Current density of free electrons	(5.4)
$j_n(x)$	Spherical Bessel function of the first kind	(5.242), Appendix C
j_ν	Emission coefficient per unit mass at frequency ν	(2.11)
$K_{\hat{a}}$	Equilibrium constant for activity	(4.78)
K_c	Equilibrium constant for concentration	(4.80)
K_p	Equilibrium constant for pressure p	(4.79)
$K_n(x)$	Modified Bessel function of the second kind and order n	(6.30) and (7.31), Appendix C
K_ν	Second angular moment of spectral radiance at frequency ν	(2.23)
$\boldsymbol{K}$	Angular momentum operator	(3.80) and (3.93)
k	Boltzmann constant	
$\boldsymbol{k}$	Complex wave vector	(5.15) and (5.17)
$\boldsymbol{k}'$	Real part of wave vector	(5.14)
$\boldsymbol{k}''$	Imaginary part of wave vector	(5.14)
L	Total angular momentum	p. 33
L	Lorenz factor	(9.38)
L_{VW}	Vleck–Weisskopf impact line profile	(7.97)
L_{ZN}	Zhevakin–Naumov line profile	(7.98)
L_ν	Line shape function	(5.60a)
$\mathcal{L}_\nu$	Line shape function (Lorentz and resonance)	(5.63) and (5.208)
l_p	Length of radiation path for a given optical depth at a given pressure	(11.20)
M	Molecular (also atomic) mass	(2.56)

(continued)

(continued)

Symbol	Description	Eq. No.
M_j	Number density of molecules of species j	(4.87)
$\boldsymbol{M}$	Magnetization (average magnetic dipole moment per unit volume)	(5.6)
$\boldsymbol{M}_{l,m}$	Vector spherical harmonic	(5.241) and (5.242)
$\mathcal{M}_i$	Mass of nucleus i in electron masses	(3.58)
$\mathcal{M}_j^{(\mathrm{I})}$	Number density of molecules of species j in ionization stage I	(4.87)
m	Mass of electron	
m_i	Mass of ion	
m_{amu}	Electron mass in atomic mass units	(3.40a)
N	Component of the total angular momentum at right angles to the internuclear axis. It represents the rotation of the nuclei alone	p. 61
N_b	Number of bound electrons per atom	(3.50)
N_o	Avogadro number	
N_e	Number of electrons per unit volume (see also ρ_e)	(3.24)
$N_\mathrm{e}(r)$	Spherically averaged electron density as a function of r (distance from the nucleus)	(3.31a)
$N_\mathrm{e}(v)$	Number of electrons with velocity v per unit volume	(5.96a) and (5.96b)
N_f	Number of free electrons per atom	(3.50)
N_I	Population of ionization stage I	(4.58)
N_i	Occupation number of level i	(2.2)
$N_i^{(\mathrm{n})}$	Occupation number of level i in a neutral atom	(3.47)
$\bar{N}_i$	Mean occupation number of level i	(3.44)
$\boldsymbol{N}_{l,m}$	Vector spherical harmonic	(5.241) and (5.243)
$\mathcal{N}$	Column number density	(7.140)
$\mathcal{N}_{\mathrm{I}i}$	Occupation number of state i in ion I	(4.64)
$\mathcal{N}_i^{\mathrm{I}}$	Number density of atoms of element i in ionization stage I	(4.85)
n	Complex refractive index	(5.19)
$\mathrm{n_r}$	Real part of refractive index	(5.19)
$\mathrm{n_i}$	Imaginary part of refractive index	(5.19)
$\hat{\boldsymbol{n}}$	Unit vector normal to a surface (Fig. 2.1)	(2.13)
n_i^*	Effective principal quantum number of level i	(3.53)
$n_\nu(\hat{\boldsymbol{\omega}})$	Number of photons of frequency ν in direction $\hat{\boldsymbol{\omega}}$	(5.54a) and (5.54b)
P_g	Gas pressure	(4.18)
P_i	Partial pressure of species i	(4.72a)
$P^{(\mathrm{c})}$	A priori probability for a configuration	(7.100)
$P_i(r)$	r times radial wave function of an electron in level i	(3.1)
$P_\mathrm{v}(R)$	R times vibrational wave function of molecule	(3.76)
$\boldsymbol{P}$	Electric polarization (average electric dipole moment per unit volume)	(5.5)
$\mathcal{P}_\nu$	Photoelectric edge distribution function	(6.3)
$\mathcal{P}_\nu(x)$	Symmetric band contour profile	(11.9)
$\mathcal{P}(\nu, \nu_\mathrm{o}, \gamma, \Gamma)$	Pressure broadened Lorentz line profile	(7.191)

$p(\cos\Theta)$	Phase function for angle between incident and scattered radiation	(2.9)
p_i	Ratio of occupation to statistical weight of state i	(2.2) and (3.41)
p_f	Probability that the final state is occupied	(6.1)
$\boldsymbol{p}$	Momentum of electron	(5.48)
$\boldsymbol{p}_\mathrm{F}$	Electron Fermi momentum	(9.43)
$p_\mathrm{lv}^{\mathrm{uv}'}$	Band strength for diatomic molecular band	(5.125)
p_R	Radial momentum	(3.68) and (3.70)
p_θ	Angular momentum	(3.69)
Q	Partition function	(4.94)
Q_el	Electronic partition function	(4.94) and (4.95)
Q_I	Partition function of ionization state I	(4.59)
Q_rot	Rotational partition function	(4.94) and (4.97)
Q_vib	Vibrational partition function	(4.94) and (4.96)
$\mathcal{Q}$	Number of nuclei in molecule	(3.56) and (3.58)
q	Number of bound levels	(3.2)
q	Number of equivalent electrons in a shell	(5.85b)
q	Autoionization line profile index	(5.160)
q	Number of electrons in a molecule	(3.56) and (3.57)
q_i, q_{ij}	Normal (generalized) coordinates	(5.112) and (5.116)
$q_{\mathrm{v}'\mathrm{v}}$	Franck–Condon factor	(5.120) and (5.122)
q_v	Space variable	(5.53), (5.54a), and (5.54b)
R	Internuclear separation in molecule	(3.60)
R_{ij}	Radiative rate between states i and j	(2.1)
R_e	Equilibrium separation of nuclei	(3.64b) and (5.109)
R_o	Universal gas constant	
$R_{\mathrm{o}n}$	Equilibrium separation of nuclei in molecule	(3.65)
R_{nl}	Radial part of wave function	(4.55a)
$\bar{R}_{\mathrm{v}'\mathrm{v}}$	R-centroid	(5.121)
R_∞	Rydberg constant	
$\boldsymbol{R}_i$	Position coordinate of nucleus i	(3.56)
$\lvert\boldsymbol{\mathcal{R}}\rvert_\mathrm{if}$	Electric dipole matrix element for a molecule from initial state i to final state f	(5.99)
r	Radius	
r_ce	Classical electron radius	(5.43)
r_D	Debye screening radius for ions	(4.61), (6.28), and (7.76)
r_De	Debye screening radius for electrons	(6.55)
r_i	Ion sphere radius for a fully ionized atom	(9.32)
r_n	Space coordinate normal to a surface	(2.16)
r_L	Lewis cutoff	(7.64)
r_o	Effective radius of atom	(4.2) and (4.4)
$\boldsymbol{r}$	Position coordinate of an electron	(5.14a), (5.14b), and (5.28)
$\boldsymbol{r}_\mathrm{e} \equiv \lvert\boldsymbol{r}(R)\rvert_\mathrm{lu}$	Electronic transition moment	(5.118)
S	Spin or multiplicity of state	(3.10)
S	Entropy	(4.19)
$S_{JK}^{J'K'}$	Hönl–London (H–L) factor	(5.101)
$S_{\mathrm{v}J}^{\mathrm{v}'J'}$	Vibration-rotation line strength	(5.100)
$S_\mathrm{v}^{\mathrm{v}'}$	Vibration part of line strength	(5.105)

(continued)

(continued)

Symbol	Description	Eq. No.
$S_J^{J'}$	Rotational factor of vibration-rotation line strength	(5.100)
S_{ij}	Transport coefficient	(9.12) and (9.13)
$\langle S \rangle$	Scattering integral	(9.55)
$\mathcal{S}(\hat{\mathcal{L}})$	Relative line strength of a line in a multiplet	(5.67)
$\mathcal{S}(\hat{\mathcal{M}})$	Relative multiplet strength of a multiplet in a transition array	(5.67)
$S(n, n')$	Electronic line strength	(5.75)
$[S_i]$	Concentration of species S_i	(4.80)
$\boldsymbol{S}$	Poynting vector	(5.35)
$\hat{s}$	Symmetry number of molecule	(4.97)
$\hat{s}_i$	Screening parameter of level i	(3.37)
T	Temperature	
T_D	Debye characteristic temperature	(9.40)
T_n	Electronic term value in molecule	(3.61b)
T_v	Period of molecular vibration	(3.68)
$T_\nu(\Delta r)$	Transmissivity at frequency ν	(2.61)
t	Time	
t_i	Energy scaling parameter	(3.48)
U	Internal energy per unit volume	(4.99)
$\bar{U}$	Energy density of electromagnetic field	(5.37)
u	Reduced photon energy	(2.7)
u_rad	Total radiation energy density	(2.48)
$u(m)$	Polarization bispinor for spin component m	(3.19)
$u_n(\boldsymbol{R}_i, \boldsymbol{r}_j)$	Electron eigenfunction for electronic state n in molecule	(3.57)
V_a	Volume of atom	(4.4)
$V_i(r)$	Potential energy for electron i	(3.14)
$\mathcal{V}$	Voigt line profile	(7.17)
$v_{nvJ}(\boldsymbol{R}_i)$	Nuclear eigenfunction for electronic state n in molecule	(3.60)
$\bar{v}$	Mean thermal speed of electron	(9.5)
x_e	Vibrational constant	(3.62)
W_i	Relativistic energy of level i	(5.246)
$W(\lvert \boldsymbol{E} \rvert)$	Holtzmark electric field distribution	(7.47)
$W_\mathrm{P}(u)$	Planck weighting function	(2.59)
$W_\mathrm{R}(u)$	Rosseland weighting function	(2.60)
w	Equivalent width of a line	(2.63)
w_if	Transition probability from initial state i to final state f	(5.45)
w_{jk}	Line coupling coefficient	(7.89)
$Y_n(x)$	Bessel function of the second kind (also known as Weber or Neumann functions) and order n	Appendix C
$Y_{l,m}$	Spherical harmonic	(3.20)
$y_n(x)$	Spherical Neuman function of order n	(5.268c), Appendix C

Z	Atomic number	
Z'	Charge number of an ion	(3.53)
Z_i^*	Energy effective charge number of level i	(3.37)
Z_i^{**}	Wave function effective charge for level i	(5.86) and (5.89)
α	Chemical potential	(3.23)
α_e	Rotational-vibrational coupling constant	(3.64a)
α_M	Molar polarizability	(5.31b)
α_p	Polarizability	(5.29)
α_i	T–F scaling factor	(3.25)
α_o	Fine structure constant	(3.11)
$\widetilde{\alpha}$	Line splitting per unit field strength	(7.70)
α_ν	Absorptivity	(2.62)
$\alpha_{\tilde{\nu}}^{\mathrm{l}}$	Linear absorption coefficient wavenumber integrated over one line (SI units: m^{-2})	(7.140)
$\alpha_{\mathrm{v}\mathrm{v}'}$	Wavenumber integrated band absorption	(7.131)
$\alpha'^{\mathrm{v}'J'}_{\mathrm{v}J}$	Absorption coefficient wavenumber integrated over a single molecular line, corrected for stimulated emission	(7.1)
$\alpha'^{\mathrm{v}'}_{\mathrm{v}}$	Absorption coefficient wavenumber integrated over rotational fine structure, corrected for stimulated emission	(7.2)
$\boldsymbol{\alpha}$	Dirac velocity matrix operator	(3.16)
$\overline{\alpha_{\tilde{\nu}}}$	Mean absorptivity wavenumber-integrated over a single line	(7.141)
β	Dirac matrix operator	(3.16)
β_i	Initial electron velocity divided by speed of light	(5.96b)
β_n	Spectroscopic constant	(3.65), (3.66a), and (3.66b)
Γ	Inelastic collision broadening half-maximum half-width (HMHW)	(7.22), (7.27), and (7.29)
Γ_C	Ion–ion Coulomb interaction parameter	(9.31)
$\widetilde{\gamma}$	Lorentz contraction factor	(5.200)
γ_i	Activity coefficient of species i	(4.75)
$\gamma_i^{(\mathrm{n})}$	Natural radiative half-maximum half-width	(5.64)
γ_s	Ratio of the averaged squares of off-diagonal to diagonal components of scattering tensor	(5.222) and (5.223)
$\gamma^{(\mathrm{n})}$	Half-maximum half-width (HMHW) for medium with refractive index n	(5.26) and (5.41)
Δ_{ni}	Quantum defect	(3.53)
δ_l	Phase shift for l-wave function	(3.21a), (3.21b), and (3.55)
ε_o	Permittivity of vacuum	(5.5)
ε	Kinetic energy of free electron	(3.22)
$\varepsilon_{\mathrm{d}j}$	Energy of formation of molecule j in an infinitely diluted gas	(4.104)
$\varepsilon_\nu(\rho, T)$	Emissivity at frequency ν, density ρ, and temperature T. See also η_ν	(2.32)
$\varepsilon(\rho, T)$	Total emissivity at density ρ and temperature T	(2.38)

(continued)

(continued)

Symbol	Description	Eq. No.
ε_{e}	Complex permittivity of medium	(5.18)
$\varepsilon_{\mathrm{e}}'$	Real part of permittivity of medium	(5.18)
$\varepsilon_{\mathrm{e}}''$	Imaginary part of permittivity of medium	(5.18)
$\varepsilon^{\mathrm{LJ}}$	Depth of Lennard–Jones intermolecular potential	(8.45b)
$\widetilde{\varepsilon}_{\nu}$	Emission coefficient per unit volume at frequency ν	(2.3)
ϵ	Complex permittivity of a medium relative to that of vacuum (dielectric function)	(5.22a) and (5.23a)
ϵ	Electron energy	
ϵ_{F}	Electron energy at the Fermi surface	(9.45)
ξ_i	Spin–orbit radial interaction for level i	(3.11)
$\xi_l(x)$	Riccati–Hankel function	(5.268b)
$\hat{\boldsymbol{\xi}}_{\wp}$	Spherical unit basis vector	(5.240)
$\eta = \alpha/(kT)$	Electron degeneracy parameter	(4.9)
η^*	Electron degeneracy parameter corrected for continuum lowering	(4.8) and (4.9)
η_i	Normal coordinate	(3.85)
η_{ν}	Emission efficiency at frequency ν; see also $\varepsilon_{\nu}(\rho, T)$	(5.257), (5.276a), and (5.276b)
Θ	Angle between incident and scattered radiation	Fig. 2.1
θ	Polar angle	Fig. 2.1
κ_{e}	Electron opacity	(9.2)
κ_{ν}	Mass extinction coefficient at frequency ν	(2.10b)
κ_{P}	Planck mean opacity	(2.57)
κ_{R}	Rosseland mean opacity	(2.58)
$\kappa_{\mathrm{P}}(\Delta u)$	Planck group mean opacity	(2.64)
κ_{t}	Total (radiative and electron) Rosseland opacity	(9.4)
$\kappa_{\mathrm{R}}(\Delta u)$	Rosseland group mean opacity	(2.65)
$\kappa_{\mathcal{T}}(\Delta u)$	Transmission group mean opacity	(2.66)
Λ_{e}	Thermal conductivity by electrons	(9.1)
$\Lambda_{\mathrm{ie}}^{\mathrm{s}}$	Electron–ion scattering mean free path	(9.5)
Λ_{L}	Lorentz gas thermal conductivity	(9.11)
Λ_{ν}	Mean free path for extinction at frequency ν	(2.10a)
Λ_{R}	Transport equivalent of photon conductivity	(9.4a)
λ_{C}	Compton wavelength	(9.33)
μ_{o}	Permeability of vacuum	(5.6)
μ_{m}	Magnetic permeability	(5.9)
μ_{r}	Reduced nuclear mass	(3.64b)
$\widetilde{\mu}_{\mathrm{r}}$	Reduced nuclear mass in electron mass units	(3.76)
μ_{a}	Linear mean radiance weighted absorption coefficient	(2.52)
μ_{f}	Linear mean flux weighted absorption coefficient	(2.51)

μ_ν	Linear extinction coefficient at frequency ν	(2.5)
μ_ν^{a}	Linear absorption coefficient at frequency ν	(2.6a)
$\mu_\nu^{\mathrm{a}'}$	Linear absorption coefficient at frequency ν corrected for stimulated emission	(2.5) and (2.6a)
μ_ν^{s}	Linear scattering coefficient at frequency	(2.5)
$\mu_\nu^{\mathcal{T}}$	Linear transport extinction coefficient at frequency ν	(2.27)
$\mu_\nu^{\mathrm{s}\mathcal{T}}$	Linear transport scattering coefficient at frequency	(2.27)
$\mu_{\mathrm{P}}(\rho, T)$	Planck mean absorption coefficient at density ρ and temperature T	(2.40)
$\mu_{\mathrm{R}}(\rho, T)$	Rosseland mean extinction coefficient at density ρ and temperature T	(2.50)
$\breve{\boldsymbol{\mu}} = e\boldsymbol{r}_{\mathrm{e}}$	Atomic electric dipole moment	(5.28)
$\breve{\boldsymbol{\mu}} = e\boldsymbol{\mathcal{R}}$	Molecular electric dipole moment	(5.99)
ν	Photon frequency	
$\tilde{\nu}$	Photon wavenumber	
ν_i	Stoichiometric coefficient of species i	(4.65)
ν_{p}	Electron plasma (or plasmon) frequency	(5.33)
ν_{pi}	Ion plasma frequency	(9.40)
ρ	Mass density	
ρ	Collision impact parameter	(7.24), (7.25), and (7.30)
ρ_{e}	Density of free electrons ($\rho_{\mathrm{e}} = eN_{\mathrm{e}}$)	(5.1)
ρ_2	Density operator	(7.96)
$\hat{\rho}$	Canonical (energy) density	(7.165)
$\hat{\rho}_{\mathrm{f}}$	Density per unit volume of final states per energy interval	(5.45) and (5.52)
σ	Stefan–Boltzmann constant	(2.37a)
σ_{e}	Electric conductivity	(5.8) and (9.16)
$\sigma_{\mathrm{ie}}^{\mathrm{s}}$	Electron–ion scattering cross section	(9.8)
σ_{p}	Plasmon scattering cross section	(5.206a) and (5.206b)
σ_{R}	Rayleigh cross section for photon scattering	(5.44)
σ_{T}	Thomson cross section for photon scattering by free electrons	(5.43)
σ'	In general, photoabsorption cross section corrected for stimulated (induced) emission under LTE conditions $\sigma' = \sigma[1 - e^{-h\nu/(kT)}]$	
$\sigma_{\mathrm{if}}^{(\mathrm{bb})}(\nu)$	Bound–bound cross section	(5.66a) and (5.66b)
$\sigma_{n_i^*, n_f'^*}^{(\mathrm{bb,BS})}$	Burgess–Seaton b–b cross section	(5.73)
$\sigma_{n_i^*}^{(\mathrm{bf,BS})}$	Burgess–Seaton b–f cross section	(5.92)
$\sigma_i^{(\mathrm{bf,K})}(\nu)$	Kramers b–f semiclassical cross section	(5.86)
$\sigma_1^{(\mathrm{bf,St})}(\nu)$	Stobbe b–f cross section for hydrogenic ions	(5.87)
$\sigma^{(\mathrm{inel})}(\upsilon)$	Inelastic collision cross section	(7.34)
$\sigma^{(\mathrm{ff})}(\nu)$	Free–free cross section	(5.93a) and (5.93b)
$\sigma^{(\mathrm{ff,K})}(\nu)$	Kramers f–f semiclassical cross section	(5.96)
σ_ν	Total extinction cross section at frequency ν	(2.10a)

(continued)

(continued)

Symbol	Description	Eq. No.
σ_ν^{s}	Total scattering cross section at frequency ν	(2.9)
$\sigma_\nu^{\mathrm{s}}(\Theta)$	Differential scattering cross section at frequency ν for phase angle Θ	(2.9)
$\sigma_{\mathrm{c}}^{\mathcal{T}}$	Transport scattering cross section including collective effects	(6.57)
σ_{ij}	Screening constant	(3.38)
$\sigma_{\mathrm{if}}^{(\mathrm{bb})}$	Bound–bound cross section	(5.66a)
σ^{LJ}	Lennard–Jones molecular diameter or range	(8.23), (8.27), and (8.44)
$\hat{\sigma}$	Matrix element for oscillator strength of a transition array	(5.67)
τ	Lifetime of a state	(5.158)
τ	Relaxation time	(9.50)
τ_ν	Optical thickness for extinction at frequency ν	(2.31)
$\tau_\nu^{\mathrm{a}'}$	Optical thickness for absorption at frequency ν	(2.31)
Φ	Azimuth angle	Fig. 2.1
$\Phi_{\kappa n\mu}$	Dirac bispinor	(3.18a) and (3.18b)
$\Phi_J(\theta, \phi, \chi)$	Rotator wave function for molecule	(3.60)
ϕ	Azimuthal angle	Fig. 2.1
$\phi(x)$	Thomas–Fermi function	(3.25b)
$\phi(\nu)$	Spectral function (see also $\phi(\nu)$)	(7.162) and (8.1)
χ_{e}	Complex electric susceptibility of medium	(5.10)
χ_{m}	Magnetic susceptibility of medium	(5.11)
χ_{I}	Ionization energy of ionization stage I	(4.58)
$\Psi(\boldsymbol{R}, \boldsymbol{r})$	Total wave function for molecule	(3.56)
Ψ_i	Dirac electron wave function	(3.16) and (3.19)
ψ	Electronic wave function	(5.50)
$\psi_l(x)$	Riccati–Bessel function	(5.268a)
$\psi_{n\mathrm{v}}(R)$	R times radial part of vibrational wave function of electronic state n	(3.60)
$\Omega_{\kappa\mu}$	Spherical spinor	(3.18a) and (3.18b)
$\hat{\boldsymbol{\omega}}$	Unit vector for direction	(2.3), Fig. 2.1
ω_{e}	Vibrational constant	(3.62) and (3.66a)
$\omega_{\mathrm{e}} x_{\mathrm{e}}$	Vibrational constant	(3.62) and (3.66b)
$\omega_{\mathrm{e}} y_{\mathrm{e}}$	Vibrational constant	(3.62)

Appendix B
Glossary and Abbreviations

Absorbance – The common logarithm ($\log_{10}$) of the reciprocal of the transmittance of a pure solvent = absorbancy = extinction.

Absorptance – 1 minus the transmittance.

Absorption – When a photon is absorbed by an atom (molecules) the atom (molecule) changes to a higher state of energy.

Absorption coefficient – If the radiative flux through a material decreases with distance l in proportion to $e^{-\mu l}$, then μ is called the absorption coefficient (= extinction coefficient).

Absorption oscillator strength – The ratio of the observed equivalent width of an absorption line to the equivalent width predicted on the basis of the classical oscillator model.

Absorptivity – The constant a in Beer's law relation $A = a \cdot l \cdot c$, where A is the absorbance, l the path length, and c the concentration of solution. Also known as absorptive power. Formerly known as absorbency index, absorption coefficient, or extinction coefficient.

Activity – The ratio of the fugacity of a state to the fugacity of the reference state.

Activity coefficient – The ratio of the fugacity to the pressure of the real gas. A measure of the deviation of a real gas from an ideal gas.

Amagat density unit – Gas molecular density in g-moles/m^3 at STP (P = 1 atmosphere and $T = 0°$C). The amagat density is unique for every gas and varies with pressure and temperature. It automatically corrects the ideal gas law for a real gas. The amagat number = $\rho/\rho_{\rm STP}$, where ρ is the measured density.

Amagat volume unit – Gas volume per 0.022 414 m^3/g-mol, the volume one g-mol of an ideal gas at STP (P = 1 atmosphere and $T = 0°$C).

AO – Atomic orbital.

APEX – Adjustable parameter exponential.

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402,
DOI 10.1007/978-1-4614-8797-5, © Springer Science+Business Media New York 2014

ATC theory – Anderson–Tsao–Curnutte theory for molecular line broadening and line coupling.

Auto-correlation function – Correlation of a function with itself. – See also correlation.

Avogadro constant – $N_o = 6.022\,141\,99 \times 10^{23}$ molecules/g-mol. – See also mole.

B–D – Bates–Damgard.

Beer–Lambert law (also known as Beer's law) – $I = I_o \exp(\sigma N l)$, where I_o is the radiance of the incident radiation, I the radiance of the transmitted radiation, σ is the total (extinction, i.e., absorption plus scattering) cross section for a single particle, N is the number density of particles, and l is the path length.

B–O – Born–Oppenheimer basis orbitals. Members of a complete set of independent orthogonal functions into which a wave function can be expanded.

CCA – Close-coupling approximation.

CCPPA – Coupled cluster polarization propagator approximation.

CEPA – Coupled electron-pair approximation.

C–G – Curtis – Godson approximation for molecular band absorption.

Chemical equilibrium – Implies that the composition does not change with time. If only one phase of matter exists (gas, liquid, or solid) then chemical equilibrium is homogeneous. If any two or all three phases are in equilibrium then chemical equilibrium is heterogeneous.

CHF – Coupled H–F.

CI – Configuration interaction.

CIA – Collision-induced absorption.

Clausius–Mosotti equation – (Mosotti also written: Mossotti) relates permittivity to polarizability. See also Lorentz–Lorenz formula.

CNDO – Complete neglect of differential overlap.

Collision parameter – $1/\sigma_{ie}^{s} = r_D/b_{90}$, the ratio of the Debye shielding length to the value of the impact parameter for which the deflection angle for scattering is 90°.

Collision logarithm – $\ln \sigma_{ie}^{s}$. See collision parameter.

Compton scattering – Inelastic (incoherent) high-energy scattering by a free electron.

Compton wavelength – $\lambda_C = h/(mc)$, where h is the Planck constant, c is the speed of light, and m id the mass of the particle. For an electron $\lambda_C = 2.426\,3 \times 10^{-12}$ m.

Conductive opacity – See electron opacity.

Correlation of two functions $f_1(t)$ and $f_2(t)$ – $C(t) = \int_{-\infty}^{\infty} f_1^*(t) f_2(t+\tau) d\tau$, where the asterisk denotes the complex conjugate.

CPA – Coupled pair approximation.

CSF – Configuration state function.

Curve of growth (Wachstumskurve) – Relates how the equivalent width of a spectral absorption (or emission) line increases with the number of atoms or molecules in their initial state producing the line as a function of optical depth or path length for a given optical depth. – See also equivalent width.

Dalton's law – At constant temperature the total pressure exerted by a mixture of gases in a definite volume is equal to the sum of the individual pressures that each gas would exert if it occupied the same total volume alone. Discovered by Cavendish (1781), announced by Dalton (1810).

DCA – Detailed configuration accounting.

DCAETS – Detailed configuration accounting with explicit term splitting.

De Broglie wavelength – $\lambda_e = h/p$, where h is the Planck constant and $p = mv$ is the momentum of the particle.

DDA – Discrete dipole approximation.

Detailed balance – The principle of detailed balance refers to the exact balance between a particular process and its inverse process in a system that is in thermodynamic equilibrium. When results of this principle are applied to a system that is not in strict thermodynamic equilibrium, then it is important that an appropriately defined thermodynamic quasi- or restricted equilibrium is applied (e.g., certain energy modes that equilibrate quickly as opposed to other energy modes that equilibrate much more slowly) so that the appropriate temperature can be defined.

DFT – Density functional theory.

Diffraction – Modification of radiation as it passes edges of opaque bodies.

Dipole polarizability – See polarizability.

Dispersion – Change of wavelength of radiation passing through a medium.

Disproportionation – Simultaneous oxidation and reduction of a substance reacting with itself to form two dissimilar molecules.

DTA – Detailed term accounting. Also referred to as DCAETS.

Effective band width – $\Delta\tilde{\nu}_{v-v'}$ corresponds to the wave numbers bounding the spectral region from which appreciable radiant energy is emitted or absorbed.

Einstein coefficient A – Spontaneous emission coefficient.

Einstein coefficient B – Coefficient for induced (stimulated) emission defined here in terms of radiation energy density per unit frequency interval.

Electron conduction opacity – See electron opacity.

Electron opacity – The measurable ability of a substance to obstruct the flow of thermal energy carried by electrons.

Emission (spontaneous) – An atom (molecule) in an excited state (energy state higher than the ground state) emits a photon without fixed phase relationship to other photons emitted by other atoms (molecules) in identically excited states.

Emission (induced) – An atom (molecule) in an excited state emits a photon of frequency ν under the action of an electromagnetic field at the same frequency. The incident and emitted photons have the same phase and the number of photons in the radiation field at frequency ν has increased by 1.

Emissivity – The ratio of radiation emitted by a surface (exitance) at a given frequency and temperature to the radiation emitted by a perfect blackbody radiator at the same frequency and temperature.

Energy density – See radiation energy density.

Enthalpy – The thermodynamic potential $H = U + PV$, where U is the internal energy, P is the pressure of the system, and V is the volume.

Entropy – A measure of the amount of energy in a physical system that *cannot* be used to do work. It also is a measure of disorder present in a system.

EOS – Equation of state.

Equilibrium – The state of a system in which the composition and properties undergo no observable changes.

Equivalent line width – The width of an imaginary line with a rectangular profile that is completely absorbing (or emitting Planckian radiance) equivalent to a real line (or molecular band) that absorbs (or emits) the same number of photons.

Exciton – A quantum of electronic excitation consisting of an electron–hole pair.

Exitance – The rate at which an extended source radiates energy *in all directions* per unit area. Units are W m^{-2}.

Fermi's "Golden Rule No. 2" – Originally formulated by Dirac (1927a). In perturbation theory the time rate for a transition of a system from initial state i to a final state f.

F–C – Franck–Condon.

Flux (radiative flux) – The rate at which energy is radiated from a source. Units are W. See also normal flux density.

Flux per unit frequency (radiative flux per unit frequency) – The rate at which energy is radiated from a source at a given frequency. Units are W Hz^{-1} See also normal flux density per unit frequency.

FOCI – First order configuration interaction.

Free energy – See Gibbs free energy and Helmholtz free energy.

Fugacity – The measure for the tendency of a gas to escape or expand. It is the pressure value needed at a given temperature to make the properties of a non-ideal gas satisfy the equation for an ideal gas, i.e., $f_i = \gamma_i P_i$, where γ_i is the fugacity coefficient and P_i is the partial pressure for component i of the gas. For an ideal gas, $\gamma_i = 1$.

Gaunt factor – Ratio of quantum mechanical to classical (Kramers or hydrogenic) photo cross section.

Gibbs free energy – A measure of the available work that can be extracted from some process operating at constant pressure. $G = H - TS$, where H is the enthalpy, T the temperature, and S the entropy.

GLFE – Global-local finite element.

HAM – Hydrogenic atoms in molecules.

Helmholtz free energy – $F = \bar{E} - TS$, where $\bar{E}$ is the mean value of the total energy at temperature T and density ρ and S is the entropy.

Heterogeneous system – A system of two or more regions of homogeneity.

H–F – Hartree–Fock.

H–F–S – Hartree–Fock–Slater.

H–L – Hönl–London.

HMHW – Half maximum half width: Half width at half of the peak of a spectral line.

HNC – Hypernetted chain theory.

Homogeneous system – A system whose properties are uniform throughout, or vary in a continuous manner.

HX – Hartree-plus-statistical-exchange.

IHNC – Improved hypernetted chain (HNC) theory.

INDO – Intermediate neglect of differential overlap.

Intensity (radiative intensity) – The radiant flux per unit solid angle emitted by a radiating source in a specific direction, $\hat{\boldsymbol{\omega}}$. Units are W sr^{-1}.

IR – Infra red.

Irradiance – Radiative power per unit area incident on a surface. Umits are W m^{-2}. If the angle of incidence is normal to the surface, then irradiance equals normal flux density.

J–W–K–B – Jeffrey–Wenzel–Kramers–Brillouin.

Kinetic equilibrium – Processes in which chemical reactions lead to products that are separated from true thermodynamic (including chemical) equilibrium by a potential barrier and the temperature is too low to overcome the barrier except at extremely low rates.

Kirchhoff's law – Expresses the general principle of detailed balance as applied to the emission and absorption of radiation.

Klein-Nishina scattering – Relativistic (inelastic, incoherent) photon scattering by a free electron at rest.

Law of mass action – The rate of an elementary reaction (defined by reduction of reactant or formation of product) is proportional to the concentration of each individual species involved in the elementary reaction.

LCAO – Linear combinations of atomic orbitals.

Line strength – Absorption coefficient integrated over frequency, wave number, or wavelength.

Lorentz–Lorenz formula – Relates the refractive index of a dilute gas to its density (temperature and pressure) and the molar refraction. See Clausius–Mosotti equation.

Lorentz gas – A plasma in which electrons only interact with ions. Electron–electron interaction is ignored.

Lorenz number – $L = 4\pi\varepsilon_{\mathrm{o}}(\pi k)^2/(3e^2) = 2.718\,215 \times 10^{-18}$ $\mathrm{J\,m^{-1}K^{-2}}$ $= 2.44 \times 10^{-8}$ $\mathrm{V^2K^{-2}}$. See Wiedemann–Franz law.

LTE – Local thermodynamic equilibrium.

LTHF – Linearized time-dependent Hartree–Fock.

Magnon – Quantized magnetic spin wave.

MBPT – Many-body perturbation theory.

MCA – Multi-configuration approximation.

MECI – Mono-excited configuration interaction.

MHD – Magnetohydrodynamic.

MIUTS – Mean ion with unfolded term splitting.

MLG – Multiple line group model for molecular band absorption.

MO – Molecular orbital.

Molal properties – Properties for which values are expressed per mole of the compound whose chemical formula is written.

Molar concentration – Number density.

Molar Gibbs free energy – The partial derivative of the Gibbs free energy with respect to $\hat{n}_i$, the number of moles of a constituent in a system. Molar Gibbs free energy is also called the partial molar Gibbs free energy or the molar chemical potential (or briefly, the chemical potential).

Molar polarizability – $\alpha_{\mathrm{M}} = \frac{\epsilon-1}{\epsilon+2}\frac{10^{-3}M}{\rho}$, where $\epsilon = \varepsilon_{\mathrm{e}}/\varepsilon_{\mathrm{o}}$.

Molar refraction – (in SI units) $R = (10^{-3}M/\rho)\cdot(\mathrm{n}^2-1)/(\mathrm{n}^2+2)$, where M is the gram-molecular weight, ρ the density, and n the refractive index.

Molar volume – The volume occupied by one mole of ideal gas at standard temperature and pressure (STP). Its value is $2.241\,4 \times 10^4$ $\mathrm{m^3/g\text{-}mol}$.

Mole (also gram-mole) – 1 g-mol = 1 gram molecular weight ($= 10^{-3}$ kg molecular weight).

Mole fraction – The number of moles of a component of a solution divided by the total number of moles of all components.

MRD – Multireference double-excitation.

NDDO – Neglect of diatomic differential overlap.

Neutrino opacity – The measurable ability of a substance to obstruct the flow of energy carried by neutrino pairs.

Normal flux density – The rate of radiative energy flow per unit area normal to the surface of a sphere enclosing the radiation source. Units are W/m^2.

Normal flux density per unit frequency – The rate of radiative energy flow at a given frequency per unit area normal to the surface of a sphere enclosing the radiation source. Units are $W/(m^2 Hz)$.

NLTE – Non-local thermodynamic equilibrium.

Occupation number – The number of electrons in a level of an atom or molecule.

ODF – Opacity distribution function.

Opacity – The measurable ability of a substance to obstruct by absorption and scattering the transmission of radiant energy. Opacity thus is the degree of non-transparency.

Optical depth – The dimensionless line integral of the absorption, scattering, or extinction coefficient along any path in a radiation transmitting medium.

Parity – Property change of a wave function when its variables are replaced by the negative of their coordinates.

Partition function – The primary quantity in statistical mechanics from which all thermodynamic quantities can be calculated.

Phonon – Quantized lattice wave.

PIA – Pressure-induced absorption. The same as collision-induced absorption (CIA).

Plasma frequency – The plasma frequency is the natural frequency of oscillation of electrons in a plasma displaced relative to the ion background.

Plasmon – Quantum of charge-density oscillations in a plasma; a charge-density wave in an electrically neutral collection of charges in which some of the charges are free to move in response to their Coulomb interaction.

Polariton – Quantum of coupled electromagnetic wave and another excitation (e.g., a phonon, plasmon, etc.).

Polarizability (dipole) – A microscopic electric property of dielectric media that relates the macroscopically observable electric susceptibility to the properties of the atom or molecule of the medium. It is a second rank tensor that in lowest order is a measure of the response (distortion) of the field strength of an electron cloud to an external field. It measures the average local polarization. Hyperpolarizability is a fourth-rank tensor in the study of nonlinear effects in atoms. It should not be confused with higher-order multipoles of the atomic charge distribution.

Polarization (atomic) – Induced displacement of an electron cloud toward the stronger atom in a molecule under the influence of an applied electric field.

Polarization (electronic) – Induced displacement of electrons relative to their nuclei under the influence of an applied electric field.

Polarization (interfacial) – Induced but limited migration of charge carriers (space-charge polarization).

Polarization (orientation) – See polarization (permanent).

Polarization (permanent) – Asymmetric charge distribution between unlike atomic partners of a molecule.

Poynting vector – $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$, where $\boldsymbol{E}$ is the electric field and $\boldsymbol{H}$ is the magnetic field. See also time-averaged Poynting vector.

QMD – Quantum Molecular Dynamics.

Radiance – The rate at which radiative energy passes through an area or is emitted from an area within a specific solid angle in a specific direction $\hat{\boldsymbol{\omega}}$. Units are W sr^{-1} m^{-2}. (In astronomy, astrophysics, and heat transfer, radiance is also incorrectly called specific intensity, or just intensity. See definition of intensity).

Radiation (or radiative) energy density – Total radiation energy in a field per unit volume and per unit frequency. It is evaluated by taking the density of states in a volume, $\rho(E)$ (our $\hat{\rho}_{\mathrm{f}}$), multiplying by the energy per state, $Nh\nu$, dividing by the volume, V, and accounting for the two polarization states by multiplying by 2.

Radiative flux – See flux.

Raoult's law – The vapor pressure of a solvent in an ideal solution equals the mole fraction of the solvent times the vapor pressure of the pure solvent.

Reflectance – The ratio of reflected flux to incident flux from a dielectric.

Reflectivity – The fraction of incident radiation that is reflected from a body.

Refraction – Change of speed of light, and hence of the wavelength and direction of radiation, associated with a change of the refractive index.

Resonance fluorescence – The two-photon process between the ground state and the first excited state.

R–H–F – Restricted Hartree–Fock.

R–K – Rydberg–Klein.

R–K–R – Rydberg–Klein–Rees.

RPA – Random phase approximation.

RPAE – Random phase approximation with exchange.

Saha ionization equation – Relates the fraction of ionized atoms in a plasma as a function of the temperature, T, and electron density of the plasma.

SCA – Statistical Configuration Accounting (see also UTA and STA).

SCEP – Self-consistent electron-pair.

SCF – Self-consistent-field.

SD – Calculation at a singles – doubles level.

SDQ – Singles – doubles quadrupole.

SHO – Simple harmonic oscillator.

SOPPA – Second order polarization propagator approximation.

SOS – Statistical opacity sampling.

Spectral irradiance – Radiative power per unit area and per unit frequency (or unit wave number) incident on a surface.

Spectral radiance – The rate at which radiative energy at a given frequency (or wavenumber) passes through an area or is emitted from an area within a specific solid angle in a specific direction $\hat{\boldsymbol{\omega}}$. Units are W sr^{-1} m^{-2} Hz^{-1} (or W sr^{-1} m^{-3}). (In astronomy, astrophysics, and heat transfer, radiance is incorrectly called specific spectral intensity, spectral intensity, or just intensity. See definition of intensity).

STA – Super transition array. A STA is the total transition array of a specific single-electron transition, including all possible contributing configurations, between a pair of superconfigurations.

State of a system – A state whose properties and composition is known.

Steady state – The *sum* of all processes producing a particular state is balanced by the *sum* of all processes destroying it, but the producing processes are not inverse of the destruction processes.

STO – Slater-type orbital.

Stoichiometric coefficient – Represents the quantitative degree of a chemical species participating in a reaction.

Strong coupling regime – The ratio of Coulomb energy of ions in a dense plasma relative to the thermal energy of the plasma, kT, is larger than one.

Superconfiguration – The collection of all ordinary configurations obtained by distributing N_i electrons to the ordinary shells of a supershell in all possible ways allowed by the Pauli exclusion principle.

TDA – Tamm–Dancoff approximation.

TDHF – Time-dependent H–F.

T–F – Thomas–Fermi.

T–F–A – Thomas–Fermi–Amaldi.

T–F–D – Thomas–Fermi–Dirac.

Thermodynamic equilibrium – Implies three different simultaneous equilibria: (1) Thermal equilibrium, for which the temperature must be the same throughout the system. (2) Mechanical equilibrium, which means no macroscopic movements within the system or of the system with respect to its surroundings. (3) Chemical equilibrium, which implies that the composition does not change with time. In thermodynamic equilibrium each process is exactly balanced by its inverse process. (See also detailed balance).

Thermodynamic process – A process in which changes in a system take place when subjected to thermodynamic examination.

Thermodynamic system – Part of the universe that is subjected to thermodynamic scrutiny.

Thomson scattering – Elastic (coherent) low-energy photon scattering by a free electron.

Time-averaged Poynting vector for harmonic fields – Radiation energy flux density.

Transition array – The totality of lines resulting from transitions between two configurations.

Transition cluster – The resulting spectrum corresponding to a one-electron transition from the lower level $(n, l, j)_{\mathrm{l}}$ to the upper level $(n, l, j)_{\mathrm{u}}$. It may contain many transition arrays.

Transmission coefficient – The ratio of the transmitted flux of radiation to the incident flux for a substance of unit thickness.

Transmissivity – The fraction of incident radiation transmitted through a body.

Transmittance – The radiant power transmitted by a body divided by the total radiant power incident upon the body (also known as transmission).

UTA – Unresolved transition array.

UV – Ultra violet.

VCI – Valence configuration interaction.

Vibrational angular momentum – A feature of linear polyatomic molecules. For CO_2, for example, the vibrational angular momentum quantum number l measures the angular rotation in units of $h/(2\pi)$, which is associated with the degenerate (bending) ν_2 vibration. l is usually written as a superscript to the corresponding vibrational quantum number, e.g., $\mathrm{v}_1\mathrm{v}_2^l\mathrm{v}_3$. (See Herzberg 1945.) Rotational energies and selection rules have l-dependencies.

V-R – Vibration–rotation.

Wiedemann–Franz law – Also known as the Wiedemann–Franz–Lorenz law, relates electric and thermal conductivity via the Lorenz number when a single, unique relaxation time can be calculated for non-relativistic electrons. See Lorenz number.

Wigner D function – Matrix representation of the finite rotation operator using spherical harmonics.

Appendix C
Some Mathematical Functions

C.1 Bessel Functions

The functions $J_p(z)$ and $Y_p(z)$ are the solutions of the first and second kind, respectively, to the Bessel differential equation

$$z^2 \frac{d^2 w}{dz^2} + z \frac{dw}{dz} + \left(z^2 - p^2\right) w = 0 \,,$$

where $z = x + iy$ and p is a real number.

C.1.1 Bessel Functions of the First, Second, and Third Kind

Bessel Functions of the First Kind

$$J_p(z) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(p + k + 1)} \left(\frac{z}{2}\right)^{p+2k} \,,$$

(parameter p is a real number, $0 < z < \infty$) .

$$= \frac{1}{\pi} \int_0^{\pi} \cos(z \sin\phi - p\phi) d\phi - \frac{\sin(p\pi)}{\pi} \int_0^{\infty} e^{-z \sinh t - pt} dt \,,$$

$(|\arg z| < \frac{\pi}{2})$.

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402,
DOI 10.1007/978-1-4614-8797-5, © Springer Science+Business Media New York 2014

$$J_n(z) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(n+k)!} \left(\frac{z}{2}\right)^{n+2k} ,$$

$$= \frac{1}{\pi} \int_0^{\pi} \cos(z \sin\phi - n\phi) d\phi , \quad (n = 0, 1, 2, \ldots) .$$

$$J_{-n}(z) = (-1)^n J_n(z) , \quad (n = 1, 2, 3, \ldots) .$$

$$\frac{\partial J_p(z)}{\partial z} = \frac{1}{2}\Big[J_{p-1}(z) - J_{p+1}(z)\Big] .$$

In particular:

$$J_0(z) = 1 - \frac{(\frac{z}{2})^2}{(1!)^2} + \frac{(\frac{z}{2})^4}{(2!)^2} - \frac{(\frac{z}{2})^6}{(3!)^2} + \ldots ,$$

$$J_1(z) = \frac{\frac{z}{2}}{1!} - \frac{(\frac{z}{2})^3}{1!2!} + \frac{(\frac{z}{2})^5}{2!3!} - \frac{(\frac{z}{2})^7}{3!4!} + \ldots ,$$

$$J_0'(z) \equiv \frac{\partial J_0(z)}{\partial z} = -J_1(z) .$$

Bessel Functions of the Second Kind (Also Called Weber or Neumann Functions)

$$Y_p(z) = \frac{J_p(z)\cos(p\pi) - J_{-p}(z)}{\sin(p\pi)} ,$$

(parameter p is a real number, $p \neq 0, 1, 2, \ldots$) ,

$$Y_p(z) = \frac{1}{\pi} \int_0^{\pi} \sin(z \sin\phi - p\phi) d\phi - \frac{1}{\pi} \int_0^{\infty} \left[e^{pt} + e^{-pt}\cos(p\pi)\right] e^{-z\sinh t} dt ,$$

$(|\arg z| < \frac{\pi}{2})$.

$$Y_n(z) = \frac{2}{\pi} \ln\left(\frac{z}{2}\right) J_n(z) - \frac{1}{\pi} \sum_{k=0}^{n-1} \frac{(n-k-1)!}{k!} \left(\frac{z}{2}\right)^{2k-n}$$

$$-\frac{1}{\pi} \sum_{k=0}^{\infty} (\psi(k+1) + \psi(k+n+1)) \frac{(-1)^k}{k!(n+k)!} \left(\frac{z}{2}\right)^{2k+n} ,$$

$$= \frac{1}{\pi}\int_0^{\pi} \sin(z\sin t - nt)dt - \frac{1}{\pi}\int_0^{\infty} \left[e^{nt} + (-1)^n e^{-nt}\right] e^{-z\sinh t}\, dt\,,$$
$$(|\arg z| < \frac{\pi}{2}\,, \quad n = 0, 1, 2, \ldots)\,,$$

where $\psi(m)$ is the digamma function: $\psi(1) = -\gamma$, $\psi(m) = -\gamma + \sum_{j=1}^{m-1}(j^{-1})$, and $\gamma = 0.577\,215\,665\ldots$ is Euler's constant.

$$Y_{-n}(z) = (-1)^n Y_n(z)\,, \quad (n = 1, 2, 3, \ldots)\,.$$
$$\frac{\partial Y_p(z)}{\partial z} = \frac{1}{2}\Big[Y_{p-1}(z) - Y_{p+1}(z)\Big]\,.$$

In particular:

$$Y_0(z) = \frac{2}{\pi}\left\{\left[\ln\left(\frac{z}{2}\right) + \gamma\right] J_0(z) + \frac{(\frac{z}{2})^2}{(1!)^2} - \frac{(1+\frac{1}{2})(\frac{z}{2})^4}{(2!)^2} + \frac{(1+\frac{1}{2}+\frac{1}{3})(\frac{z}{2})^6}{(3!)^2} - \ldots\right\},$$
$$Y_0'(z) \equiv \frac{\partial Y_0(z)}{\partial z} = -Y_1(z).$$

Bessel Functions of the Third Kind (Also Called Hankel Functions)

$$H_p^{(1)}(z) = J_p(z) + i\,Y_p(z)\,,$$
$$H_p^{(2)}(z) = J_p(z) - i\,Y_p(z)\,,$$
$$H_{-p}^{(1)}(z) = e^{p\pi i} H_p^{(1)}(z)\,,$$
$$H_{-p}^{(2)}(z) = e^{-p\pi i} H_p^{(2)}(z)\,, \quad \text{(parameter } p \text{ is a real number)}\,.$$
$$H_n(z) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(n+k)!}\left(\frac{z}{2}\right)^{n+2k}\,, \quad (n = 0, 1, 2, \ldots)\,.$$
$$= \frac{1}{\pi}\int_0^{\infty} \cos(z\sin\phi - n\phi)d\phi$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(z\sin\phi - n\phi)}d\phi\,.$$

C.1.2 Modified Bessel Functions (Also Called Basset Functions) of the First and Second Kind

The functions $I_p(z)$ and $K_p(z)$ are solutions of the first and second kind, respectively, to the modified Bessel differential equation

$$z^2 \frac{d^2w}{dz^2} + z\frac{dw}{dz} - \left(z^2 + p^2\right) w = 0\,,$$

where $z = x + iy$ and p is a real number.

Modified Bessel Functions of the First Kind

$$I_p(z) = \sum_{k=0}^{\infty} \frac{1}{k!\Gamma(p+k+1)} \left(\frac{z}{2}\right)^{p+2k}, \quad \text{(parameter } p \text{ is a real number)}.$$

$$I_n(z) = \sum_{k=0}^{\infty} \frac{1}{k!(n+k)!} \left(\frac{z}{2}\right)^{n+2k}, \quad (n = 0, 1, 2, \ldots)\,.$$

$$\begin{aligned} I_n(z) &= e^{-in\pi/2} J_n(ze^{i\pi/2})\,, \quad (-\pi < \arg z \leq \frac{\pi}{2})\,, \\ &= e^{i3n\pi/2} J_n(ze^{-i3\pi/2})\,, \quad (\frac{\pi}{2} < \arg z \leq \pi)\,, \\ &= \frac{1}{\pi}\int_0^{\pi} e^{z\cos\phi}\cos(n\phi)d\phi\,. \end{aligned}$$

$$I_{-n}(z) = I_n(z)\,, \quad (n = 1, 2, 3, \ldots)\,.$$

In particular:

$$I_0(z) = 1 + \frac{(\frac{z}{2})^2}{(1!)^2} + \frac{(\frac{z}{2})^4}{(2!)^2} + \frac{(\frac{z}{2})^6}{(3!)^2} + \ldots\,,$$

$$I_1(z) = \frac{z}{2} + \frac{(\frac{z}{2})^3}{1!2!} + \frac{(\frac{z}{2})^5}{2!3!} + \frac{(\frac{z}{2})^7}{3!4!} + \ldots\,,$$

$$I_0'(z) \equiv \frac{\partial I_0(z)}{\partial z} = I_1(z)\,.$$

Modified Bessel Functions of the Second Kind

$$K_p(z) = \frac{\pi[I_{-p}(z) - I_p(z)]}{2\sin(p\pi)}, \quad \text{(parameter } p \text{ is a real number)}.$$

$$K_p(z) = \frac{\pi}{2\sin(p\pi)}\Big[\sum_{k=0}^{\infty}\frac{1}{k!(n+k)!}\left(\frac{z}{2}\right)^{-n+2k} - \sum_{k=0}^{\infty}\frac{1}{k!(n+k)!}\left(\frac{z}{2}\right)^{n+2k}\Big],$$

$$K_n(z) = \frac{i\pi}{2}e^{in\pi/2}H_n^{(1)}(ze^{i\pi/2}), \quad (-\pi < \arg z \le \frac{\pi}{2}),$$

$$= -\frac{i\pi}{2}e^{-in\pi/2}H_n^{(2)}(ze^{-i\pi/2}), \quad (-\frac{\pi}{2}\arg z \le \pi).$$

$$K_{-n}(z) = K_n(z), \quad (n = 1, 2, 3, \ldots).$$

$$\frac{\partial K_p(z)}{\partial z} = \frac{1}{2}\Big[K_{p-1}(z) + K_{p+1}(z)\Big].$$

In particular:

$$K_0(z) = -\Big[\ln\left(\frac{z}{2}\right) + \gamma\Big]I_0(z) + \frac{(\frac{z}{2})^2}{(1!)^2} + \frac{(1+\frac{1}{2})(\frac{z}{2})^4}{(2!)^2} + \frac{(1+\frac{1}{2}+\frac{1}{3})(\frac{z}{2})^6}{(3!)^2} + \ldots.$$

$$K_1(z) = \frac{1}{z} + \frac{z}{4}\left[2\gamma - 1 + \frac{1}{8}\left(2\gamma - \frac{5}{2}\right)z^2 + \frac{1}{192}\left(2\gamma - \frac{10}{3}\right)z^4 + \ldots\right]$$

$$+\frac{z}{2}\ln\frac{z}{2}\left(1 + \frac{z^2}{8} + \frac{z^4}{192} + \ldots\right)$$

$$K_0'(z) \equiv \frac{\partial K_0(z)}{\partial z} = -K_1(z).$$

$$\lim_{z\to 0} zK_1(z) \to 1,$$

$$\lim_{z\to\infty} K_1(z) \to \left(\frac{\pi}{2z}\right)^{1/2}.$$

C.1.3 Spherical Bessel Functions

The functions $j_n(z)$ and $y_n(z)$ are the solutions of the first and second kind, respectively, to the Bessel differential equation

$$z^2 \frac{d^2 w}{dz^2} + 2z \frac{dw}{dz} + \left[z^2 - n(n+1)\right] w = 0\,,$$

where $z = x + iy$ is a real number and n are integers.

Spherical Bessel Function of the First Kind

$$j_n(z) = \sqrt{\frac{\pi}{2z}} J_{n+1/2}(z)$$

In particular:

$$\begin{aligned}
j_0(\rho) &= \frac{\sin(\rho)}{\rho}\,,\\
j_1(\rho) &= \frac{\sin(\rho)}{\rho^2} - \frac{\cos(\rho)}{\rho}\,,\\
j_2(\rho) &= \left(\frac{3}{\rho^2} - 1\right)\frac{\sin\rho}{\rho} - \frac{3\cos\rho}{\rho^2}\,,\\
j_3(\rho) &= \left(\frac{15}{\rho^3} - \frac{6}{\rho}\right)\frac{\sin\rho}{\rho} - \left(\frac{15}{\rho^2} - 1\right)\frac{\cos\rho}{\rho}\,.
\end{aligned}$$

Spherical Bessel Function of the Second Kind

$$y_n(z) = \sqrt{\frac{\pi}{2z}} Y_{n+1/2}(z)$$

In particular:

$$\begin{aligned}
y_0(\rho) &= -\frac{\cos(\rho)}{\rho}\,,\\
y_1(\rho) &= -\frac{\cos(\rho)}{\rho^2} - \frac{\sin(\rho)}{\rho}\,,
\end{aligned}$$

$$y_2(\rho) = \left(-\frac{3}{\rho^2} + 1\right)\frac{\cos\rho}{\rho} - \frac{3\sin\rho}{\rho^2}\,,$$
$$y_3(\rho) = \left(-\frac{15}{\rho^3} + \frac{6}{\rho}\right)\frac{\cos\rho}{\rho} - \left(\frac{15}{\rho^2} - 1\right)\frac{\sin\rho}{\rho}\,.$$

Spherical Bessel Functions of the Third Kind (Spherical Hankel Functions)

$$h_n^{(1)}(\rho) = j_n(\rho) + i y_n(\rho)\,,$$
$$h_n^{(2)}(\rho) = j_n(\rho) - i y_n(\rho)\,.$$

In particular:

$$h_0^{(1)}(\rho) = \frac{e^{i\rho}}{i\rho}\,,$$
$$h_1^{(1)}(\rho) = -\frac{e^{i\rho}}{\rho}\left(1 + \frac{i}{\rho}\right)\,,$$
$$h_2^{(1)}(\rho) = \frac{i\,e^{i\rho}}{\rho}\left(1 + \frac{3i}{\rho} - \frac{3}{\rho^2}\right)\,.$$

C.2 Binomial Function (Hypergeometric Distribution)

$$f(x) = \frac{\binom{M}{x}\binom{N-M}{n-x}}{\binom{N}{n}}\,,$$

where

$$\binom{M}{x} \equiv \frac{M!}{x!\,(M-x)!}\,, \quad (0 \le x \le M)\,.$$

Here $f(x)$ is the probability of obtaining exactly x elements of one kind and $n - x$ elements of another, if n elements are chosen at random without replacement from a finite population containing N elements of which M are of the first kind and $N - M$ are of the second kind.

C.2.1 Binomial Distribution

When there are exactly two mutually exclusive outcomes of a trial: "success" and "failure," the binomial distribution gives the probability of observing x successes in N trials, with the probability of success on a single trial denoted by p. The binomial probability function is

$$P(x, p, N) = \binom{N}{x} p^x (1-p)^{(N-x)}, \quad (x = 0, 1, 2, \ldots, N).$$

The binomial cumulative probability function is

$$F(x, p, N) = \sum_{i=0}^{x} \binom{N}{i} p^i (1-p)^{(N-i)}.$$

C.3 Fermi Integrals

C.3.1 Non-relativistic Fermi Integrals

$$\begin{aligned}
F_k(\eta) &\equiv \frac{1}{\Gamma(k+1)} \int_0^\infty \frac{x^k}{e^{x-b\eta}+1} dx, \\
F_k'(\eta) &\equiv \frac{\partial}{\partial \eta} I_k(\eta) \\
&= \frac{1}{\Gamma(k+1)} \int_0^\infty x^k \frac{\partial}{\partial \eta} \left(\frac{1}{e^{x-\eta}+1} \right) dx \\
&= -\frac{1}{\Gamma(k+1)} \int_0^\infty x^k \frac{\partial}{\partial x} \left(\frac{1}{e^{x-\eta}+1} \right) dx \\
&= -x^k \frac{1}{e^{x-\eta}+1} \Big|_0^\infty + k \int_0^\infty \frac{x^{k-1}}{e^{x-\eta}+1} dx \\
&= k F_{k-1}(\eta).
\end{aligned}$$

In particular:

$$\frac{\partial}{\partial \eta} F_{1/2}(\eta) = F_{-1/2}(\eta),$$

For additional information and tabulations see Rhodes (1950), Dingle (1957), and Wyller (1973).

Approximations

$$
\begin{aligned}
F_{1/2}(\eta) &= \frac{2}{3}\eta^{3/2}\left(1+\frac{1.23}{\eta^2}\right), \quad (\eta > 30)\,,\\
F_{1/2}(\eta) &= \frac{2}{3}\eta^{3/2}\left(1+\frac{1.23}{\eta^2}+\frac{1.25}{\eta^4}\right), \quad (4 \le \eta \le 30)\,,\\
F_{1/2}(\eta) &= \left(0.008\eta^3+0.187\eta^2+0.525\eta+0.678\right)\\
&\quad +\left(-0.012\eta^2+0.019\eta-0.009\right)|\eta|\,, \quad (-2 \le \eta < 4)\,,\\
F_{1/2}(\eta) &= 0.8862e^{\eta}-0.3133e^{2\eta}+0.569e^{3\eta}\,, \quad (-28 < \eta < -2)\,,\\
F_{1/2}(\eta) &= e^{(\eta-0.12078223)}\,, \quad (\eta \le -28)\,,\\
F_{3/2}(\eta) &= \frac{3}{4}\pi^{1/2}e^{\eta}(1-0.167764e^{\eta}+0.064150027e^{2\eta}-0.03125e^{3\eta}\\
&\quad +0.017885431e^{4\eta}-0.011340229e^{5\eta}+0.00771356158e^{6\eta})\,,\\
&\quad (\eta \le -2)\,,\\
F_{3/2}(\eta) &= 0.1758009896+\frac{3}{2}(0.6513262112+0.678091\eta+0268098335\eta^2\\
&\quad +0.05636582666\eta^3+0.00469520575\eta^4-0.00047150892\eta^5\\
&\quad -.0001066017995\eta^6)\,, \quad (-2 < \eta \le 0)\,,\\
F_{3/2}(\eta) &= 1.152790306+\frac{3}{2}(0.678091\eta+0.26819\eta^2+0.0556078333\eta^3\\
&\quad +0.005151675\eta^4-0.001202982\eta^5+0.00008173300002\eta^6)\,,\\
&\quad (0 < \eta \le 3)\,,\\
F_{3/2}(\eta) &= 10.35369867+\frac{3}{2}(-6.168596892+0.757064709\eta+0.1961444\eta^2\\
&\quad +0.0901841666\eta^3-0.0042073325\eta^4+0.00016516628\eta^5\\
&\quad -0.000003032951667\eta^6)\,, \quad (3 < \eta \le 10)\,,\\
F_{3/2}(\eta) &= 134.270211-(134.2701846+0.4\eta^{5/2}+2.467401\eta^{1/2}\\
&\quad -0.7102746\eta^{-3/2}-2.771862428\eta^{-7/2}-44.13000364\eta^{-11/2}\\
&\quad -1{,}641.825466\eta^{-15/2})\,, \quad (10 < \eta \le 10^5)\,,\\
F_{3/2}(\eta) &= \frac{2}{5}\eta^{5/2}\,, \quad (10^5 < \eta)\,.
\end{aligned}
$$

For additional information and other approximations see McDougall and Stoner (1938).

C.3.2 Relativistic Fermi Integrals

$$F_k^{(R)}(\eta, T') = \frac{1}{\Gamma(k+1)} \int_0^\infty \frac{x^k (1 + T'x)(1 + \frac{1}{2}T'x)^{1/2}}{e^{x-\eta} + 1} dx \,,$$

where $T' \equiv kT/(mc^2)$.

$$\lim_{T' \to 0} F_k^{(R)}(\eta, T') = F_k(\eta) \,,$$

C.4 Hermite Polynomials

The Hermite differential equation is

$$\frac{d^2 w}{dx^2} - 2x \frac{dw}{dx} + 2nw = 0 \,.$$

The Hermite polynomials are given by Rodrigues' formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \,,$$

$$H_n(x) = n! \sum_{k=0}^{n/2} \frac{(-1)^k}{k!(n-2k)!} (2x)^{n-2k} \,.$$

In particular:

$$\begin{aligned}
H_0(x) &= 1 \,, \\
H_1(x) &= 2x \,, \\
H_2(x) &= 4x^2 - 2 \,, \\
H_3(x) &= 8x^3 - 12x \,, \\
H_4(x) &= 16x^4 - 48x^2 + 12 \,, \\
H_5(x) &= 32x^5 - 160x^3 + 120x \,.
\end{aligned}$$

For additional information see Morse and Feshbach (1953).

C.5 Generalized Laguerre Polynomials

$$L_n^\lambda(z) = \sum_{k=0}^{n} \frac{(-1)^k}{k!} \binom{n+\lambda}{n-\lambda} z^k \,.$$

In particular:

$$\begin{aligned}
L_0^\lambda(z) &= 1\,,\\
L_1^\lambda(z) &= -z + \lambda + 1\,,\\
L_2^\lambda(z) &= \frac{z^2}{2} - (\lambda+2)z + \frac{(\lambda+2)(\lambda+1)}{2}\,,\\
L_3^\lambda(z) &= -\frac{z^3}{6} + \frac{(\lambda+3)z^2}{2} - \frac{(\lambda+2)(\lambda+3)z}{2} + \frac{(\lambda+1)(\lambda+2)(\lambda+3)}{6}\,.
\end{aligned}$$

C.6 Legendre Polynomials

C.6.1 Unassociated Legendre Polynomials

The Legendre differential equation

$$(1-x^2)\frac{d^2w}{dx^2} - 2x\frac{dw}{dx} + l(l+1)w = 0\,,$$

or

$$\frac{d}{dx}\left[(1-x^2)\frac{dw}{dx}\right] + l(l+1)w = 0\,,$$

where l is real, is a special case of the Associated Legendre equation (see Sect. C.6.2) with $m = 0$. Legendre polynomials are given by Rodrigues' formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n\,.$$

$$\begin{aligned}
P_n(z) &= \frac{1}{2^n}\sum_{k=0}^{n/2}(-1)^k \binom{n}{k}\binom{2n-2k}{n} z^{n-2k}\\
&= \frac{1}{2^{2n}}\sum_{k=0}^{n}\binom{2k}{n}\binom{2n-2k}{n-k}\cos[(n-2k)\arccos z]\,, \qquad (l \text{ is integer})\,.
\end{aligned}$$

In particular:

$$
\begin{aligned}
P_0(x) &= 1\,,\\
P_1(x) &= x\,,\\
P_2(x) &= \frac{1}{2}\cdot(3x^2-1)\,,\\
P_3(x) &= \frac{1}{2}(5x^3-3x)\,,\\
P_4(x) &= \frac{1}{8}(35x^4-30x^2+3)\,,\\
P_5(x) &= \frac{1}{8}(63x^5-70x^3+15x)\,,\\
P_6(x) &= \frac{1}{16}(231x^6-315x^4+105x^2-5)\,.
\end{aligned}
$$

For $x = \cos\theta$:

$$
\begin{aligned}
P_0(\cos\theta) &= 1\,,\\
P_1(\cos\theta) &= \cos\theta\,,\\
P_2(\cos\theta) &= \frac{1}{4}[3\cos(2\theta)+1]\,,\\
P_3(\cos\theta) &= \frac{1}{8}[5\cos(3\theta)+3\cos\theta]\,,\\
P_4(\cos\theta) &= \frac{1}{64}[35\cos(4\theta)+20\cos(2\theta)+9]\,,\\
P_5(\cos\theta) &= \frac{1}{128}[63\cos(5\theta)+35\cos(3\theta)+30\cos\theta]\,,\\
P_6(\cos\theta) &= \frac{1}{512}[231\cos(6\theta)+126\cos(4\theta)+105\cos(2\theta)+50]\,.
\end{aligned}
$$

C.6.2 Associated Legendre Polynomials

The Legendre associated differential equation is

$$
(1-x^2)\frac{d^2w}{dd^2} - 2x\frac{dw}{dx} + \left[l(l-1) + \frac{m^2}{1-x^2}\right]w = 0\,.
$$

Associated Legendre functions of the first kind are given by

$$\begin{aligned} P_l^m(x) &= (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x) \\ &= \frac{(1-x^2)^{m/2}}{2^l l!}\frac{d^{m+l}}{dx^{m+l}}(x^2-1)^l\,. \\ P_l^{-m}(x) &= (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x)\,. \end{aligned}$$

In particular:

$$\begin{aligned} P_0^0(x) &= 1\,, \\ P_1^0(x) &= x\,, \\ P_1^1(x) &= -(1-x^2)^{1/2}\,, \\ P_2^0(x) &= \frac{1}{2}(3x^2-1)\,, \\ P_2^1(x) &= -3x(1-x^2)^{1/2}\,, \\ P_2^2(x) &= 3(1-x^2)\,, \\ P_3^0(x) &= \frac{1}{2}x(5x^2-3)\,, \\ P_3^1(x) &= -\frac{3}{2}(1-5x^2)(1-x^2)^{1/2}\,, \\ P_3^2(x) &= 15x(1-x^2)\,, \\ P_3^3(x) &= -15(1-x^2)^{3/2}\,, \end{aligned}$$

For $x = \cos\theta$:

$$\begin{aligned} P_0^0(\cos\theta) &= 1\,, \\ P_1^0(\cos\theta) &= \cos\theta\,, \\ P_1^1(\cos\theta) &= -\sin\theta\,, \\ P_2^0(\cos\theta) &= \frac{1}{2}(3\cos^2\theta-1)\,, \\ P_2^1(\cos\theta) &= -3\cos\theta\sin\theta\,, \\ P_2^2(\cos\theta) &= 3\sin^2\theta\,, \\ P_3^0(\cos\theta) &= \frac{1}{2}(5\cos^3\theta-3\cos\theta)\,, \end{aligned}$$

$$P_3^1(\cos\theta) = -\frac{3}{2}(5\cos^2 - 1)\sin\theta\,,$$
$$P_3^2(\cos\theta) = 15\cos\theta\sin^2\theta\,,$$
$$P_3^3(\cos\theta) = -15\sin^3\theta\,,$$

C.7 Coulomb Corrections to Pressure and Entropy of an Ideal Gas of Ions

Semi-empirical fits to data by Brush et al. (1966) for the Coulomb correction (see van Horn 1971).

$$\frac{(P - P_o)V}{NkT} = -0.113\Gamma^{3/2}\left[\frac{1}{(1 + 0.142\Gamma)^{1/2}} + \frac{1.54}{(1 + 0.575\Gamma)^{3/2}}\right],$$
$$\frac{(S - S_o)}{Nk} = -\ln\left[1 + \frac{\Gamma^{3/2}}{2\sqrt{3}}\left(0.015 + \frac{0.585}{1 + \Gamma^{1/2}} + \frac{0.400}{1 + 1.308\Gamma^{3/2}}\right)\right],$$

P_o and S_o are the pressure and entropy of a perfect gas of N ions in a box of volume V at temperature T. $\Gamma = (Ze)^2/(4\pi\epsilon_o r_o kT)$ is the ratio of the Coulomb interaction energy relative to the thermal energy kT, and r_o is the ion sphere radius.

C.8 Spherical Harmonics

C.8.1 Scalar Spherical Harmonics

$$Y_l^m(\theta,\phi) = (-1)^m\left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\phi}\,, \quad (-l < m < l)\,.$$
$$Y_{l'}^{m'*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi)\,,$$

where superscript * indicates the complex conjugate.

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_{l'}^{m'*}(\theta,\phi)Y_l^m(\theta,\phi)\sin\theta d\theta d\phi = \delta_{ll'}\delta_{mm'}\,.$$

In particular:

$$
\begin{aligned}
Y_0^0(\theta,\phi) &= \sqrt{\frac{1}{4\pi}}\,,\\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta\,,\\
Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}\,,\\
Y_2^0(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta-1\right)\,,\\
Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}\,,\\
Y_2^{\pm2}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{\pm 2i\phi}\,.
\end{aligned}
$$

C.8.2 Vector Spherical Harmonics

$$
\begin{aligned}
\boldsymbol{M}^{(z)}_{\substack{\text{odd,}\\\text{even,}}mn} &= \pm\frac{m}{\sin\theta}\begin{matrix}\cos(m\phi)\\ \sin(m\phi)\end{matrix} P_n^m(\cos\theta) z_n(\rho)\hat{\boldsymbol{e}}_\theta - \begin{matrix}\sin(m\phi)\\ \cos(m\phi)\end{matrix}\frac{dP_n^m(\cos\theta)}{d\theta} z_n(\rho)\hat{\boldsymbol{e}}_\phi\,,\\
\boldsymbol{N}^{(z)}_{\substack{\text{even,}\\\text{odd,}}mn} &= \frac{z_n(\rho)}{\rho}\begin{matrix}\cos(m\phi)\\ \sin(m\phi)\end{matrix} n(n+1)P_n^m(\cos\theta)\hat{\boldsymbol{e}}_r\\
&\quad + \begin{matrix}\cos(m\phi)\\ \sin(m\phi)\end{matrix}\frac{dP_n^m(\cos\theta)}{d\theta}\frac{1}{\rho}\frac{d[\rho z_n(\rho)]}{d\rho}\hat{\boldsymbol{e}}_\theta\\
&\quad \mp \frac{m\sin(m\phi)}{m\cos(m\phi)}\frac{P_n^m(\cos\theta)}{\sin\theta}\frac{1}{\rho}\frac{d[\rho z_n(\rho)]}{d\rho}\hat{\boldsymbol{e}}_\phi\,,
\end{aligned}
$$

here z_n stands for any one of four spherical Bessel functions of the first kind j_n, the second kind y_n, or the third kind (Hankel functions) $h_n^{(1)}$, or $h_n^{(2)}$. $\hat{\boldsymbol{e}}_\theta$ and $\hat{\boldsymbol{e}}_\phi$ are unit vectors.

Appendix D
Units, Conversion Factors, and Fundamental Physical Constants for Opacities

We present units, conversion factors, and some fundamental physical constants that are useful for opacity calculations. Many of these and others can be found on the Web at http://physics.nist.gov/cgi-bin/cuu. Updates on physical constants can be found at http://physics.nist.gov/cuu/Constants/Index.html.

Atomic mass constant:

$$10^{-3} \times \frac{M(^{12}\mathrm{C})}{12} \frac{1}{N_\mathrm{o}} = 1.660\,538\,86 \times 10^{-27}\ \mathrm{kg}$$

$$10^{-3} \times \frac{M(^{12}\mathrm{C})}{12} \frac{1}{N_\mathrm{o}} c^2 = 1.492\,417\,90 \times 10^{-10}\ \mathrm{J} = 931.494\,043\ \mathrm{MeV}$$

Atomic unit of length (first Bohr radius of hydrogen), area, and volume:

$$a_\mathrm{o} = \frac{\varepsilon_\mathrm{o} h^2}{\pi m e^2} = \frac{\alpha_\mathrm{o}}{4\pi R_\infty} = 5.291\,772\,09 \times 10^{-11}\ \mathrm{m}$$

$$\pi a_\mathrm{o}^2 = 8.797\,355\,37 \times 10^{-21}\ \mathrm{m}^2$$

$$\frac{4\pi}{3} a_\mathrm{o}^3 = 6.207\,146\,61 \times 10^{-31}\ \mathrm{m}^3$$

Atomic unit of time:

$$\tau_\mathrm{o} = (4\pi R_\infty c)^{-1} = 2.418\,884\,326 \times 10^{-17}\ \mathrm{s}$$

Avogadro constant:

$$N_\mathrm{o} = 6.022\,141\,5 \times 10^{23}\ \text{atoms (g-mol)}^{-1}$$

Bohr radius: see atomic unit of length

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402,
DOI 10.1007/978-1-4614-8797-5, © Springer Science+Business Media New York 2014

Boltzmann constant:

$$k = 1.380\,650\,5 \times 10^{-23}\ \mathrm{J\ K^{-1}} = 8.617\,343\ \times 10^{-5}\ \mathrm{eV\ K^{-1}}$$
$$\frac{k}{h} = 2.083\,664\,4 \times 10^{10}\ \mathrm{Hz\ K^{-1}}$$
$$\frac{k}{hc} = 69.503\,564\ \mathrm{m^{-1}\ K^{-1}}$$

Classical electron radius:

$$r_{\mathrm{ce}} = \frac{e^2}{4\pi\varepsilon_{\mathrm{o}} mc^2} = \alpha_{\mathrm{o}}^2 a_{\mathrm{o}} = 2.817\,940\,29 \times 10^{-15}\ \mathrm{m}$$

Compton wavelength:

$$\lambda_{\mathrm{C}} = \frac{h}{mc} = 2\pi\alpha_{\mathrm{o}} a_{\mathrm{o}} = \frac{\alpha^2}{2R_\infty} = 2.426\,310\,22 \times 10^{-12}\ \mathrm{m}$$

Einstein B_{lu} coefficient for radiation density per unit frequency interval at the frequency of the absorption line in terms of the oscillator strength:

$$B_{\mathrm{lu}} = \frac{e^2}{4h\nu m\varepsilon_{\mathrm{o}}} f_{\mathrm{lu}}$$

Conversion factors to Einstein B_{lu} coefficient for radiation density per unit frequency interval at the frequency of the absorption line $[\mathrm{s^{-1}(Jm^{-3}Hz^{-1})^{-1}}]$ from:

B_{lu} coefficient for radiation density per unit wavelength interval at the wavelength of the absorption line $[\mathrm{s^{-1}(Jm^{-3}m^{-1})^{-1}}]$: ν^2/c,

B_{lu} coefficient for radiance per unit wavelength interval at the wavelength of the absorption line $[\mathrm{s^{-1}(Wm^{-2}sr^{-1}m^{-1})^{-1}}]$: $\nu^2/(4\pi)$,

B_{lu} coefficient for radiance per unit frequency interval at the frequency of the absorption line $[\mathrm{s^{-1}(Wm^{-2}sr^{-1}Hz^{-1})^{-1}}]$: $c/(4\pi)$.

Electric charge:

$$1\ \mathrm{C} = 1\ \mathrm{F} \times 1\ \mathrm{V}$$

Electric dipole moment:

$$1\ \text{debye} \equiv 10^{-18}\ \text{esu cm} = 3.335\,64 \times 10^{-30}\ \mathrm{C\ m}$$
$$ea_{\mathrm{o}} = 8.478\,353\,07 \times 10^{-30}\ \mathrm{C\ m}$$
$$e \times 1\ \text{Å} = 1.602\,176\,53 \times 10^{-29}\ \mathrm{C\ m}$$
$$e \times 1\ \mathrm{nm} = 1.602\,176\,53 \times 10^{-28}\ \mathrm{C\ m}$$

Electric quadrupole moment:

$$ea_o^2 = 4.486\,551\,23 \times 10^{-40}\ \mathrm{C\ m^2}$$

Electric potential:

$$1\ \mathrm{V} = 1\ \mathrm{J/C}$$

Electron mass:

$$m = 9.109\,382 \times 10^{-31}\ \mathrm{kg} = 5.485\,799 \times 10^{-4}\ \mathrm{amu}$$
$$(N_o 10^3 m)^{-1} = 1{,}822.89\ \mathrm{amu/electron}$$

Electron mass energy equivalent:

$$mc^2 = 8.187\,104 \times 10^{-14}\ \mathrm{J} = 0.510\,998\,9\ \mathrm{MeV} = 2/\alpha_o^2\ \mathrm{ryd}$$

Electron plasma frequency:

$$\nu_p = \left(\frac{N_e e^2}{4\pi^2 m \varepsilon_o}\right)^{1/2} = 8.978\,662\,8\ N_e^{1/2}\ \mathrm{Hz}$$

Elementary charge:

$$e = 1.602\,176\,5 \times 10^{-19}\ \mathrm{C}$$
$$\frac{e^2}{4\pi\varepsilon_o} = 2.307\,077\,2 \times 10^{-28}\ \mathrm{J\ m}$$
$$\frac{e^2}{4\pi\varepsilon_o} \cdot \frac{\pi}{mc} = 2.654\,009 \times 10^{-6}\ \mathrm{m^2 s}$$

Energy (see also Hartree and Rydberg units):

$$1\ \mathrm{J} = 6.241\,509\,48 \times 10^{18}\ \mathrm{eV} = 4.587\,425\,13 \times 10^{17}\ \mathrm{ryd}$$
$$1\ \mathrm{F} = 1\ \mathrm{C/V}$$
$$1\ \mathrm{C\ V} = 1\ \mathrm{J}$$
$$1\ \mathrm{eV} = 1.602\,176\,53 \times 10^{-19}\ \mathrm{J}$$
$$1\ \mathrm{eV}/ch = 8.065\,544\,45 \times 10^5\ \mathrm{m^{-1}}$$
$$1\ \mathrm{ryd} = 2.179\,872\,1 \times 10^{-18}\ \mathrm{J}$$
$$1\ \mathrm{ryd}/ch = 1.097\,367\,7 \times 10^7\ \mathrm{m^{-1}}$$
$$1\ \mathrm{eV}/k = 1.160\,450\,5 \times 10^4\ \mathrm{K}$$

Fine structure constant:

$$\alpha_o = \frac{e^2}{2\varepsilon_o hc} = 7.297\,352\,54 \times 10^{-3}$$
$$\alpha_o^{-1} = 137.035\,999\,7$$

Hartree unit of energy (= 2 Rydberg units of energy):

$$2R_\infty hc = \frac{e^2}{4\pi\varepsilon_o a_o} = 4.359\,744\,17 \times 10^{-18}\ \text{J} = 27.211\,384\,5\ \text{eV}$$

Ion plasma frequency

$$\nu_{pi} = \left(\frac{N_i (Ze)^2}{4\pi^2 \varepsilon_o m_i}\right)^{1/2} = 5.160\,682 \times 10^{12} \frac{Z}{A} \rho^{1/2}\ \text{Hz}$$

Loschmidt constant:

$$N_L = \frac{N_o}{V_M} = 2.686\,777 \times 10^{25}\ \text{m}^{-3}\ \ (\text{at } T = 273.15\ \text{K},\ P = 101.325\ \text{kPa}).$$

The Loschmidt constant must be used with care, because sometimes (e.g., see CODATA definitions) it is defined at $P = 100\,\text{kPa}$. In that case $N_L = 2.651\,646 \times 10^{25}\ \text{m}^{-3}$. In this book it is always defined for $P = 1$ atm.

Molar gas constant:

$$R_o = kN_o = 8.314\,472\ \text{J (g-mol)}^{-1}\text{K}^{-1}$$

Molar volume of ideal gas:

$$\frac{R_o T}{P} = V_M = 22.413\,996 \times 10^{-3}\ \text{m}^3\text{(g-mol)}^{-1}\ \ (\text{at } T = 273.15\ \text{K},\ P = 101.325\ \text{kPa})$$

Permeability of vacuum:

$$\mu_o = 4\pi \times 10^{-7}\ \text{N A}^{-2} = 1.256\,637\,061\,4\ldots \times 10^{-6}\ \text{N A}^{-2}\ \ (\text{exact})$$

Permittivity of vacuum:

$$\varepsilon_o = 1/(4\pi \times 10^{-7} c^2) = 8.854\,187\,817\ldots \times 10^{-12}\ \text{F m}^{-1}\ \ (\text{exact})$$
$$\frac{1}{4\pi\varepsilon_o} = 8.987\,551\,178\,8 \times 10^9\ \text{V m C}^{-1}$$

Planck constant:

$$h = 6.626\,068\,96 \times 10^{-34}\ \text{J s} = 4.135\,667\,33 \times 10^{-15}\ \text{eV s}$$
$$hc = 1.986\,455\,44 \times 10^{-25}\ \text{J m}$$

Plasma frequency see: electron or ion plasma frequency
Proton mass:

$$1.672\,621\,71 \times 10^{-27}\ \text{kg}$$

Radiation constant (first):

$$c_1 = 2\pi hc^2 = 3.741\,771\,38 \times 10^{-16}\ \text{W m}^2$$

Radiation constant (second):

$$c_2 = \frac{hc}{k} = 1.438\,775\,2 \times 10^{-2}\ \text{m K}$$

Rydberg constant for infinite mass:

$$R_\infty = \left(\frac{e^2}{4\pi\varepsilon_\text{o}}\right)^2 \frac{2\pi^2 m}{h^2 c} = 1.097\,373\,156\,852\,5 \times 10^7\ \text{m}^{-1}$$

Rydberg frequency:

$$R_\infty c = 3.289\,841\,960\,360 \times 10^{15}\ \text{Hz}$$

Rydberg unit of energy:

$$R_\infty hc = \frac{e^2}{8\pi\varepsilon_\text{o} a_\text{o}} = 2.179\,872\,09 \times 10^{-18}\ \text{J} = 13.605\,692\,3\ \text{eV} \equiv 1\ \text{ryd}$$

Speed of light in vacuum:

$$c = 2.997\,924\,58 \times 10^8\ \text{m s}^{-1} \quad \text{(exact)}$$

Stefan constant:

$$a_\text{S} = 4\frac{\sigma}{c} = 7.565\,767\,4 \times 10^{-16}\ \text{J m}^{-3}\ \text{K}^{-4} = 4.722\,180\,9 \times 10^3\ \text{eV m}^{-3}\ \text{K}^{-4}$$

Stefan-Boltzmann constant:

$$\sigma = \frac{2\pi^5 k^4}{15h^3c^2} = 5.670\,400 \times 10^{-8}\ \mathrm{W\ m^{-2}K^{-4}} = 3.539\,186 \times 10^{11}\ \mathrm{eV\ m^{-2}\,K^{-4}s^{-1}}$$

Thomson cross section:

$$\sigma_\mathrm{T} = \frac{8\pi}{3} r_\mathrm{ce}^2 = 6.652\,458\,73 \times 10^{-29}\ \mathrm{m^2}$$

Conversion of dimensionless polarizability ($\alpha_\mathrm{p}/4\pi\varepsilon_\mathrm{o}a_\mathrm{o}^3$) to polarizability in F m^2 (or C m^2 V^{-1}):

$$4\pi\varepsilon_\mathrm{o}a_\mathrm{o}^3 = 1.648\,777\,274 \times 10^{-41}\ \mathrm{F\,m^2}$$

Conversion of polarizability in F m^2 to molar polarizability in m^3/(g-mol):

$$\frac{N_\mathrm{o}}{3\varepsilon_\mathrm{o}} = 2.267\,153\,7 \times 10^{34}\ \mathrm{m^3/F\,m^2(g\text{-}mol)}$$

Conversion of polarizability in SI units to cgs units in cm^3:

$$\alpha_\mathrm{p}[\mathrm{cm^3}] = \frac{100h}{4\pi\,\varepsilon_\mathrm{o}}\frac{\alpha}{h}\ [\mathrm{Hz/(V/cm)^2}] = 5.955\,213\,79 \times 10^{-22}\frac{\alpha}{h}\ [\mathrm{Hz/(V/cm)^2}]$$

Conversion from wavelength in vacuum to energy:

$$E = \frac{hc}{\lambda_\mathrm{vac}} = 1.986\,455\,44 \times 10^{-16}\ \mathrm{J}\ \ (\lambda_\mathrm{vac}\ \text{in nm})$$

$$E = \frac{hc}{\lambda_\mathrm{vac}} = \frac{1{,}239.848\,0}{\lambda_\mathrm{vac}}\ \mathrm{eV}\ \ (\lambda_\mathrm{vac}\ \text{in nm})$$

$$E = \frac{hc}{\lambda_\mathrm{vac}} = \frac{91.127\,164}{\lambda_\mathrm{vac}}\ \mathrm{ryd}\ \ (\lambda_\mathrm{vac}\ \text{in nm})$$

Appendix E
Some Relevant Websites

The intent here is not to give an exhaustive list of websites, but to give a short list of some websites relevant for opacities.

Atomic Physics Codes:
Codes based on R. D. Cowan's The Theory of Atomic Structure and Spectra:
http://www.tcd.ie/Physics/people/Cormac.McGuinness/Cowan/

Atomic, Molecular, and Electron Collisions:
http://aphysics2.lanl.gov/tempweb/lanl/
http://www.ruf.rice.edu/~atmol/index.html

Databases:
http://www.nist.gov/srd/
HIgh resolution TRANsmission (HITRAN) database:
http://www.cfa.harvard.edu/HITRAN

Electron Conductivity for Stellar Plasmas:
http://www.ioffe.rssi.ru/astro/conduct/conduct.html

Electron Impact Cross Sections for Ionization and Excitation:
http://physics.nist.gov/PhysRefData/Ionization/Xsection.html
International Atomic Energy Agency:
http://www-amdis.iaea.org/databases.html
National Institute for Fusion Science, Data and Planning Center (Nagoya, Japan):
http://dbshino.nifs.ac.jp

EOS and Associated Data for Materials in the Sesame Library:
http://t1web.lanl.gov
http://www.lanl.gov/orgs/t/t1.shtml
First-time users click on "Sesame registration."

Gaussian Basis Sets are Described in GAUSSIAN-98 User's Guide:
http://www.gaussian.com/

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402,
DOI 10.1007/978-1-4614-8797-5,

Kinetics Databases:
http://kinetics.nist.gov/kinetics/
http://kinetics.nist.gov/solution/
http://www.udfa.net

Rate Coefficients for Radiative Processes:
Solar and blackbody radiation:
http://phidrates.space.swri.edu
Photodissociation and photoionization of astrophysically relevant molecules:
http://home.strw.leidenuniv.nl/~ewine/photo/

Materials Libraries:
http://www.codata.org/
Click on "Databases", then click on "International Register of Materials Database Managers."

Opacities:
Opacity (astrophysical and general): http://aphysics2.lanl.gov/opacity/lanl/
Opacity Project (TOPbase):
http://cdsweb.u-strasbg.fr/topbase.html
Livermore (OPLIB):
http://www-phys.llnl.gov/Research/OPAL/opal.html
http://www.cita.utoronto.ca/~boothroy/kappa.html
http://www.physast.uga.edu/ugamop
Low-temperature opacities:
http://webs.wichita.edu/physics/opacity/
Programs and data for CIA opacities:
http://www.astro.ku.dk/~aborysow/programs/

Physics Data Libraries:
http://www.fas.harvard.edu/~planets/planetarylinks.html

Thermodynamic Data:
http://kinetics.nist.gov/janaf
Chemical Equilibrium:
http://www.grc.nasa.gov/WWW/CEAWeb/ceaRequestForm.htm

Units, Conversion Factors, and Fundamental Physical Constants:
http://physics.nist.gov/cuu/Constants/index.html
http://spintronics.inha.ac.kr/unit.pdf
http://newton.ex.ac.uk/research/qsystems/collabs/constants.html
http://qft.iqfr.csic.es/PhysRefData/codata86/codata86.html

References

Numbers in brackets indicate the chapters in which the references are cited.

Abdallah Jr., J., Clark, R. E. H. (1991): 'X-ray transmission calculations for an aluminum plasma.' *J. Appl. Phys.* **69**, 23–26. [13]

Abdallah Jr., J., Clark, R. E. H., Cowan, R. D. (1988): 'Theoretical Atomic Physics Code Development. I. CATS: Cowan Atomic Structure Code.' Los Alamos National Laboratory report LA-11436-M. [3]

Abraham, Z., Iben, I. (1971): 'More solar models and neutrino fluxes.' *Astrophys. J.* **170**, 157–163. [11]

Abramowitz, M., Stegun, I. A. (1964/1972): *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. NBS Applied Mathematics Series **55**, U.S. Dept. Commerce, Washington, DC. Tenth printing, December 1972, with corrections. [5, 8]

Acton, A. P., Aickin, R. G., Bayliss, N. S. (1936): 'The continuous absorption spectrum of bromine: A new interpretation.' *J. Chem. Phys.* **4**, 474–479. [6]

Adam, J. C., Serveniere, A. G., Laval, G. (1983): 'Instabilities induced by resonant absorption of an electromagnetic wave in an inhomogeneous plasma.' *J. Phys., Colloque C2 Suppl.* **44**, 171–179. [5]

Adelman, S. J., Wiese, W. L.(1995): *Astrophysical applications of powerful new databases: Joint discussion no. 16 of the 22nd General Assembly of the IAU.* Astronomical Society of the Pacific, San Francisco. [1, 13]

Aden, A. L. (1951): 'Electromagnetic scattering from spheres with sizes comparable to the wavelength.' *J. Appl. Phys.* **22**, 601–605. [5]

Aden, A. L., Kerker, M. (1951): 'Scattering of electromagnetic waves from two concentric spheres.' *J. Appl. Phys.* **22**, 1242–1246. [5]

Adey, A. W. (1956): 'Scattering of electromagnetic waves by coaxial cylinders.' *Can. J. Phys.* **34**, 510–520. [5]

Adler-Golden, S. M., Langhoff, S. R., Bauschlicher Jr., C. W., Carney, G. D. (1985): 'Theoretical calculation of ozone vibrational infrared intensities.' *J. Chem. Phys.* **83**, 255–264. [5]

Ågren, H., Arneberg, R., Müller, J., Manne, R. (1984): 'X-ray emission of the nitrogen molecule following photon or electron impact. A theoretical study using configuration-interaction wavefunctions.' *Chem. Phys.* **83**, 53–67. [5]

Ahlrichs, R. (1979): 'Many body perturbation calculations and coupled electron pair models.' *Comp. Phys. Comm.* **17**, 31–45. [5]

Ahlrichs, R., Scharf, P. (1987): 'The coupled pair approximation.' *Adv. Chem. Phys.* **67**, 501–537. [3, 5]

Akhiezer, A. I., Berestetskii, V. B. (1965): *Quantum Electrodynamics*. 2^{nd} ed., (Engl. trans.), Interscience, New York. [3, 5]

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402, DOI 10.1007/978-1-4614-8797-5,

Albrecht, A. C. (1961): 'On the theory of Raman intensities.' *J. Chem. Phys.* **34**, 1476–1484. [5]
Alder, K., Bohr, A., Huus, T., Mottelson, B., Winther, A. (1956): 'Study of nuclear structure by electromagnetic excitation with accelerated ions.' *Rev. Mod. Phys.* **28**, 432–542. [7]
Alexander, D. R. (1975): 'Low-temperature Rosseland opacity tables.' *Astrphys. J. Suppl. Ser.* **29**, 363–374. [6]
Alexander, D. R., Ferguson, J. W. (1994a): 'Improvements in the computation of grain opacities.' In *Molecules in the Stellar Environment.* Ed. U. G. Jørgensen, Springer-Verlag, Berlin, p. 149–162. [6]
Alexander, D. R., Ferguson, J. W. (1994b): 'Low-temperature Rosseland opacities.' *Astrphys. J.* **437**, 879–891. [6, 7]
Alexander, D. R., Johnson, H. R., Rypma, R. L. (1983): 'Effect of molecules and grains on Rosseland mean opacities.' *Astrophys. J.* **272**, 773–780. [6, 7]
Alhassid, Y., Gürsey, F., Iachello, F. (1983): 'Group theory approach to scattering.' *Ann. Phys. (NY)* **148**, 346–380. [5]
Allard, F., Hauschildt, P. H. (1995): 'Model atmospheres for M (sub)dwarf stars. I. The base model grid.' *Astrophys. J* **445**, 433–450. [14]
Allard, F., Hauschildt, P. H., Alexander, T. R., Tamanai, A., Schweitzer, A. (2001): 'The limiting affects of dust in brown dwarf atmospheres.' *Astrophys. J.* **556**, 357–372. [14]
Allen, C. W. (1963): *Astrophysical Quantities*. 2^{nd} ed., The Athlone Press, University of London, and Humanities Press, Inc., New York. [5]
Allen, S. J. M. (1935): 'Mean values of the mass absorption coefficient of the elements.' In *X-Rays in Theory and Experiment*, Appendix IX. Eds. A. H. Compton and S. K. Allison; D. van Nostrand Co., Inc., Princeton, NJ, Toronto, New York, London, p. 799. Also in *Handbook of Chemistry and Physics*. 53^{rd} ed., p. E-123. [5]
Allison, A. C., Dalgarno, A. (1971); 'Continuity at the dissociation threshold in molecular absorption.' *J. Chem. Phys.* **55**, 4342–4344. [5]
Ambarzumian, V. A. (1936): 'The effect of absorption lines on the radiative equilibrium of the outer layers of stars.' *Publ. Obs. Astronom. Univ. Leningrad* **6**, 7–18. [7]
Amos, R. D. (1987a): 'Molecular property derivatives.' *Adv. Chem. Phys.* **67**, 99–153. [3, 5]
Amos, R. D. (1987b): 'Geometries, harmonic frequencies and infrared and Raman intensities for H_2O, NH_3, and CH_4.' *J. Chem. Soc. Faraday Trans. 2*, **83**, 1595–1607. [5]
Amusia, M. Y.(1996a): 'Many-body theory of atomic structure and processes.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 287–300. [3, 5]
Amusia, M. Y.(1996b): 'Atoms as many-body systems.' *Phys. Rep.* **264**, 7–26. [5]
Amus'ya, M. Ya., Cherepkov, N. A., Chernysheva, L. V. (1971): 'Cross section for the photoionization of noble-gas atoms with allowance for multielectron correlations.' *Zh. Eksper. Teor. Fiz.* **60**, 160–174 (*Sov. Phys. - JETP* **33**, 90–96). [5]
Anderson, P. W. (1949): 'Pressure broadening in the microwave and infra-red regions.' *Phys. Rev.* **76**, 647–661. [7]
Andresen, P. (1986a): 'Classification of pump mechanism for astronomical OH masers and a maser model for the H_2O photodissociation pump mechanism.' *Astron. Astrophys.* **154**, 42–54. [5]
Andresen, P. (1986b): 'Possible pump mechanisms for astronomical OH masers.' *Comments At. Mol. Phys.* **18**, 1–9. [5]
Andresen, P., Schinke, R. (1987): 'Dissociation of water in the first absorption band: A model system for direct photodissociation.' In *Molecular Photodissociation Dynamics*. Eds. M. N. R. Ashfold and J. E. Baggott; Royal Society of Chemistry, Burlington House, Piccadilly, London, p. 61–113. [5]
Anicich, V. G. (1993): 'A survey of bimolecular ion – molecule reactions for use in modeling the chemistry of planetary atmospheres, cometary comae, and interstellar clouds.' *Astrophys. J. Suppl. Ser.* **84**, 215–315. [4]
Ansbacher, A. (1959): 'A note on the overlap integral of two harmonic oscillator wave functions.' *Z. Naturforsch. A* **14**, 889–892. [5]

Appell, P., Kampe de Feriet, J. (1926): *Fonctions Hypergeometrique et Hyperspherique Polynomes d'Hermite.* Gauthier-Villars, Paris. [5]

Arking, A., Grossman, K. (1972): 'Influence of line shape and band structure on temperatures in planetary atmospheres.' *J. Atmos. Sci.* **29** 937–949. [7]

Armstrong, B. H. (1964a): 'Apparent positions of photoelectric edges and the merging of spectral lines.' *J. Quant. Spectr. Rad. Transfer* **4**, 207–214. [5, 7]

Armstrong, B. H. (1964b): 'Research on opacity of high-temperature air.' *J. Quant. Spectr. Rad. Transfer* **4**, 731–736. [1]

Armstrong, B. H. (1967): 'Spectrum line profiles: The Voigt function.' *J. Quant. Spectr. Rad. Transfer* **7**, 61–88. [5, 7]

Armstrong, B. H., Purdum, K. L. (1966): 'Extended use of the Coulomb approximation: Mean powers of r, a sum rule, and improved transition integrals.' *Phys. Rev.* **150**, 51–59. [7]

Armstrong, B. H., Sokoloff, J., Nicholls, R. W., Holland, D. H., Meyerott, R. E. (1961): 'Radiative properties of high temperature air.' *J. Quant. Spectr. Rad. Transfer* **1**, 143–162. [1]

Armstrong, B. H., Johnston, R. R., Kelly, P. S. (1965): 'The atomic line contribution to the radiation absorption coefficient of air.' *J. Quant. Spectr. Rad. Transfer* **5**, 55–65. [11]

Armstrong, B. H., Johnston, R. R., Kelly, P. S., DeWitt, H. E., Brush, S. G. (1967): 'Opacity of high-temperature air.' *Prog. High Temp. Phys. Chem.* **1**, 139–242. [1, 4, 5, 7]

Asano, S. (1979): 'Light scattering properties of spheroidal particles.' *Appl. Optics* **18**, 712–723. [5]

Asano, S., Yamamoto, G. (1975): 'Light scattering by a spheroidal particle.' *Appl. Optics* **14**, 29–49. [5]

Asinovsky, Z. J., Kirillin, Z. V., Kobsev, G. A. (1970): 'Study of the continuum radiation of nitrogen plasmas.' *J. Quant. Spectr. Rad. Transfer* **10**, 143–164. [13]

Auman Jr., J. (1966): 'The infrared opacity of hot water vapor.' *Astrophys. J. Suppl. Ser.* **14**, 171–206. [7]

Avilova, I. V., Biberman, L. M., Vorobjev, V. S., Zamalin, V. M., Kobzev, G. A., Lagar'kov, A. N., Mnatsakanian, A. Ch., Norman, G. E. (1969a): 'Optical properties of heated air – I. Basic procedures of spectral characteristics.' *J. Quant. Spectr. Rad. Transfer* **9**, 89–111. [1]

Avilova, I. V., Biberman, L. M., Vorobjev, V. S., Zamalin, V. M., Kobzev, G. A., Lagar'kov, A. N., Mnatsakanian, A. Ch., Norman, G. E. (1969b): 'Optical properties of heated air – II. Integrated characteristics.' *J. Quant. Spectr. Rad. Transfer* **9**, 113–122. [1]

Bacher, R. F., Goudsmit, S. (1934): 'Atomic energy relations. I.' *Phys. Rev.* **46**, 948–969. [3]

Back, C. A., Perry, T. S., Bach, D. R., Wilson, B. G., Iglesias, C. A., Landen, O. L., Davidson, S. J., Crowley, B. J. B. (1997): 'Opacity measurements: Extending the range and filling in the gaps.' *J. Quant. Spectr. Rad. Transfer* **58**, 415–425. [13]

Bahcall, J. N., Huebner, W. F., Lubow, S. H., Parker, P. D., Ulrich, R. K. (1982): 'Standard solar models and the uncertainties in predicted capture rates of solar neutrinos.' *Rev. Mod. Phys.* **54**, 767–799. [13]

Balasubramanian, K., Pitzer, K. S. (1987): 'Relativistic quantum chemistry.' *Adv. Chem. Phys.* **67**, 287–320. [3]

Balescu, R. (1960): 'Irreversible processes in ionized gases.' *Phys. Fluids* **3**, 52–63. [9]

Balescu, R. (1961): 'Approach to equilibrium of a quantum plasma.' *Phys. Fluids* **4**, 94–99. [9]

Baranger, M. (1958): 'Problem of overlapping lines in the theory of pressure broadening.' *Phys. Rev.* **111**, 494–504. [7]

Baranger, M. (1962): 'Spectral line broadening in plasmas.' In *Atomic and Molecular Processes*. Ed. D. R. Bates; Academic Press, New York, London, p. 493–548. [7]

Baranov, V. I. (2000): 'Parametric method in the theory of vibronic spectra of polyatomic molecules: Absorption and fluorescence spectra and structure of styrene in the excited state.' *Optika Spectrosk.* **88**, 216–223 (Russian); *Opics Spectrosc.* **88** 182–189 (English). [5]

Baranov, v. I., Gribov, L. A., Zelent'sov, D. Yu (1996): 'Refined approach for matrix element calculations in the theory of electronic-vibration spectra of polyatomic molecules.' *J. Mol. Struct.* **376**, 475–493. [5]

Bardsley, J. N. (1968): 'Configuration interaction in the continuum states of molecules.' *J. Phys. B* **1**, 349–364. [5]

Barfield, W. D. (1977): 'Theoretical study of equilibrium nitrogen plasma radiation.' *J. Quant. Spectr. Rad. Transfer* **17**, 471–482. [10]

Barfield, W. D., Huebner, W. F. (1976): 'On the calculation of scattering cross sections from absorption cross sections.' *J. Quant. Spectr. Rad. Transfer* **16**, 27–34. [5]

Barfield, W. D., Koontz, G. D., Huebner, W. F. (1972): 'Fits to new calculations of photoionization cross sections for low-Z elements.' *J. Quant. Spectr. Rad. Transfer* **12**, 1409–1433; **13**, 87. [5, 6, 12]

Barin, I. (1995): *Thermochemical Data of Pure Substances.* VCH Publishers, New York, N.Y. [4]

Baron, E., Hauschildt, P. H. (1998): 'Parallel implementation of the PHOENIX generalized stellar atmosphere program. II. Wavelength parallelization.' *Astrophys. J.* **495**, 370–376. [14]

Baron, E., Hauschildt, P. H., Nugent, P., Branch, D. (1996): 'Non-local thermodynamic equilibrium effects in modeling supernovae near maximum light.' *Mon. Not. Roy. Astron. Soc.* **283**, 297–315. [14]

Bar-Shalom, A., Oreg, J., Glodstein, W. H., Shvarts, D., Zigler, A. (1989): 'Super-transition arrays: A model for the spectral analysis of hot, dense plasma.' *Phys. Rev. A* **40**, 3183–3193. [7, 13]

Bar-Shalom, A., Oreg, J., Glodstein, W. H., (1994): 'Configuration interaction in LTE spectra of heavy elements.' *J. Quant. Spectr. Rad. Transfer* **51**, 27–39. [7, 13]

Bar-Shalom, A., Oreg, J., Goldstein, W. H., (1995a): 'Effect of configuration widths on the spectra of local thermodynamic equilibrium plasmas.' *Phys. Rev. E* **51**, 4882–4890. [7]

Bar-Shalom, A., Oreg, J., Seely, J. F., Feldman, U., Brown, C. M., Hammel, B. A., Lee, R. W., Back, C. A. (1995b): 'Interpretation of hot and dense absorption spectra of a near-local-thermodynamic-equilibrium plasma by the super-transition-array method.' *Phys. Rev. E* **52**, 6686–6691. [7, 13]

Bartlett, R. J., Musial, M. (2007): 'Coupled-cluster theory in quantum chemistry.' *Rev. Mod. Phys.* **79**, 291–352. [3]

Bates, D. R. (1946): 'An approximate formula for the continuous radiative absorption cross-section of the lighter neutral atoms and positive and negative ions.' *Mon. Not. Roy. Astron. Soc.* **106**, 423–431. [5]

Bates, D. R., Damgaard, A. (1949): 'The calculation of the absolute strengths of spectral lines.' *Phil. Trans. Roy. Soc. London, Ser. A* **242**, 101–122. [3, 5, 7]

Bauche, J., Bauche-Arnoult, C. (1990): 'Statistical properties of atomic spectra.' *Comp. Phys. Rep.* **12**, 1–28. [7]

Bauche, J., Bauche-Arnoult, C., Klapisch, M., Mandelbaum, P., Schwob, J.-L. (1987): 'Quenching of transition arrays through configuration mixing.' *J. Phys. B* **20** 1443–1450. [7]

Bauche-Arnoult, C., Bauche, J. (1992): 'Statistical approach to the spectra of plasmas.' *Phys. Scripta* **T40**, 58–64. [7]

Bauche-Arnoult, C., Bauche, J., Klapisch, M. (1978): 'Mean wavelength and spectral width of transition arrays in x-uv atomic spectra.' *J. Opt. Soc. Am.* **68** 1136–1139. [7]

Bauche-Arnoult, C., Bauche, J., Klapisch, M. (1979): 'Variance of the distributions of energy levels and of the transition arrays in atomic spectra.' *Phys. Rev. A* **20** 2424–2439. [7]

Bauche-Arnoult, C., Bauche, J., Klapisch, M. (1982): 'Variance of the distributions of energy levels and of the transition arrays in atomic spectra. II. Configurations with more than two open shells.' *Phys. Rev. A* **25** 2641–2646. [7]

Bauche-Arnoult, C., Bauche, J., Klapisch, M. (1984): 'Asymmetry of $l^{N+1} - l^N l'$ transition array patterns in ionic spectra.' *Phys. Rev. A* **30** 3026–3032. [7]

Bauche-Arnoult, C., Bauche, J., Klapisch, M. (1985): 'Variance of the distribution of energy levels and of the transition arrays in atomic spectra. III. Case of spin-orbit-split arrays.' *Phys. Rev. A* **31** 2248–2259. [7]

Bauer, A., Godon, M., Carlier, J., Ma, Q. (1995): 'Water vapor absorption in the atmospheric window at 239 GHz.' *J. Quant. Spectr. Rad. Transfer* **53**, 411–423. [7]

Bauer, A., Godon, M., Carlier, J., Gamache, R. R. (1996): 'Absorption of a H_2O–CO_2 mixture in the atmospheric window at 239 GHz.' *J. Mol. Spectr.* **176**, 45–57. [7]

Bauer, A., Godon, M., Carlier, J., Gamache, R. R. (1998): 'Continuum in the windows of the water vapor spectrum. Absorption of H_2O–Ar at 239 Ghz and linewidth calculations.' *J. Quant. Spectr. Rad. Transfer* **59**, 273–285. [7]

Bauschlicher Jr., C. W., Langhoff, S. R., Taylor, P. R. (1990): 'Accurate quantum chemical calculations.' *Adv. Chem. Phys.* **77**, 103–162. [3]

Beck, D. R., Nicolaides, C. A. (1978): 'Theory of electronic structure of excited states in small systems with numerical applications to atomic states.' In *Excited States in Quantum Chemistry: Theoretical and Experimental Aspects of the Electronic Structure and Properties of the Excited States in Atoms, Molecules and Solids*. Eds. C. A. Nicolaides and D. R. Beck; D. Reidel Publ. Co., Dordrecht, Boston, London, p. 105–142. [5]

Beck, D. R., Nicolaides, C. A. (1982): 'Specific correlation effects in inner-electron photoelectron spectroscopy.' *Phys. Rev. A* **26**, 857–862. [5]

Becke, A. D. (1992): 'Density-functional thermochemistry. I. The effect of the exchange-only gradient correction.' *J. Chem. Phys.* **96**, 2155–2160. [3]

Becke, A. D. (1993): 'Density-functional thermochemistry. III. The role of exact exchange.' *J. Chem. Phys.* **98**, 5648–5652. [3]

Behrens, H., Ebel, G., Lück, W., Luksch, P., Müller, H.-W. (1985): 'Data compilations in physics.' *Physics Data* 3–5. [6]

Behringer, J. (1958): 'Zur Theorie des Resonanz-Raman-Effektes.' *Z. Elektrochem.* **62**, 906–914. [5]

Bely, O. (1966): 'Quantum defect theory. III. Electron scattering by He^+.' *Proc. Phys. Soc. (London)* **88**, 833–842. [3]

Bely, O., Griem, H. R. (1970): 'Quantum-mechanical calculation for the electron-impact broadening of the resonance lines of singly ionized magnesium.' *Phys. Rev. A* **1**, 97–105. [7]

Benedict, W. S., Kaplan, L. D. (1959): 'Calculation of line widths in H_2O - N_2 collisions.' *J. Chem. Phys.* **30**, 388–399. [7]

Benedict, W. S., Kaplan, L. D. (1964): 'Calculation of the line widths in H_2O – H_2O and H_2O – O_2 collisions.' *J. Quant. Spectr. Rad. Transfer* **4**, 453–469. [7]

Benedict, W. S., Gailar, N., Plyler, E. K. (1956): 'Rotation–vibration spectra of deuterated water vapor.' *J. Chem. Phys.* **24**, 1139–1165. [5]

Benedict, W. S., Herman, R., Moore, G. E., Silverman, S. (1957): 'Infrared line and band strengths and dipole moment functions in HCl and DCl.' *J. Chem. Phys.* **26**, 1671–1677. [7]

Ben-Reuven, A. (1966): 'Impact broadening of microwave spectra.' *Phys. Rev.* 145, 7–22. [7]

Berestetskii, V. B., Lifshitz, E. M., Pitaevskii, L. P. (1971): *Relativistic Quantum Theory*. Pergamon Press, Oxford, New York. [5]

Berger, R., Klessinger, M. (1997): 'Algorithm for exact counting of energy levels of spectroscopic transitions at different temperatures.' *J. Comp. Chem.* **18**, 1312–1319. [7]

Berger, R., Fischer, C., Klessinger, M. (1998): 'Calculation of the vibronic fine structure in electronic spectra at high temperatures. I. Benzene and pyrazine.' *J. Phys. Chem. A* **102**, 7157–7167. [5, 7, 13]

Bernstein, J., Dyson, F. J. (1959): 'The continuous opacity and equations of state of light elements at low densities.' General Atomic report GA-848. [11]

Berrington, K. (1997a): *The Opacity Project, Volume 2*. Inst. of Physics Publishing, Bristol, Philadelphia. [1, 3, 4]

Berrington, K. A. (1997b): 'The opacity and iron projects - an overview.' In *Photon and Electron Collisions with Atoms and Molecules.* Eds. P. G. Burke and C. J. Joachain. Plenum Press; New York, London, p. 297–312. [1, 7]

Berrington, K. A., Eissner, W., Saraph, H. E., Seaton, M. J., Storey, P. J. (1987a): 'A comparison of close-coupling calculations using UCL and QUB codes.' *Comp. Phys. Comm.* **44**, 105–119. [3]

Berrington, K. A., Burke, P. G., Butler, K., Seaton, M. J., Storey, P. J., Taylor, K. T., Yan, Y. (1987b): 'Atomic data for opacity calculations: II. Computational methods.' *J. Phys. B* **20**, 6379–6397. [3]

Bethe, H. A. (1964): *Intermediate Quantum Mechanics*. W. A. Benjamin, Inc., New York, Amsterdam. [3]

Bethe, H. A., Salpeter, E. E. (1957): *Quantum Mechanics of One- and Two-Electron Atoms*. Springer-Verlag, Berlin, Göttingen, Heidelberg. [3, 5, 7, 12]

Biberman, L. M., Norman, G. E. (1967): 'Continuous spectra of atomic gases and plasma.' Soviet Phys. Usp. (Engl. trans.) **10**, 52–90. [1, 5]

Biedenharn, L. C., Blatt, J. M., Rose, M. E. (1952): 'Some properties of the Racah and associated coefficients.' *Rev. Mod. Phys.* **24**, 249–257. [6]

Biedenharn, L. C., Louck, J. D., Carruthers, P. A. (1981): *Angular Momentum in Quantum Physics. Theory and Application.* Encyclopedia of Mathematics and its Applications. **8**, Addison-Wesley Publishing Co., Reading, MA, London, Amsterdam, Don Mills, Ontario, Sydney, Tokyo. [6]

Bielińska-Waż, D., Karwowski, J. (1998): 'Statistical theory of vibronic spectra: The intensity distributions.' *J. Quant. Spectr. Rad. Transfer* **59**, 39–51. [7]

Biermann, L. (1933): 'Stellar Atmospheres.' *Göttinger Nachrichten, Math. Phys. Klasse* **3**, 297–315 and 350–358. [2]

Biggs, F., Lighthill, R. (1972): 'Analytical Approximations for Photon-Atom Differential Scattering Cross Sections Including Electron Binding Effects.' Sandia Laboratory report SC-RR-72 0659. [5]

Billingsley II, F. P., Krauss, M. (1974): 'MCSCF calculation of the dipole moment function of CO $X^1\Sigma^+$.' *J. Chem. Phys.* **60**, 4309–4316. [5]

Birnbaum, G. (1994): 'A memory function approach to the shape of pressure broadened molecular bands.' *Mol. Phys.* **81**, 519–532. [7]

Birnbaum, G., Cohen, E. R. (1976a): 'Theory of line shape in pressure-induced absorption.' *Can. J. Phys.* **54**, 593–602. [8, 13]

Birnbaum, G., Cohen, E. R. (1976b): 'Determination of molecular multipole moments and potential function parameters of non-polar molecules from far infra-red spectra.' *Mol. Phys.* **32**, 161–167. [8]

Birnbaum, G., Cohen, E. R. (1976c): 'Theory of line shape in pressure-induced absorption.' *Icarus* **54**, 593–602. [8]

Birnbaum, G., Borysow, A. (1991): 'On the problem of detailed balance and model line shapes in collision-induced rotovibrational bands: H_2-H_2 and H_2-He.' *Mol. Phys.* **73**, 57–68. [8]

Birnbaum, G., Guillot, B., Bratos, S. (1982): 'Theory of collision-induced line shapes – absorption and light scattering at low density.' *Adv. Chem. Phys.* **51**, 49–112. [8]

Birnbaum, G., Chu, S.-I., Dalgarno, A., Frommhold, L., Wright, E. L. (1984): 'Theory of collision-induced translation-rotation spectra: H_2 – He.' *Phys. Rev. A* **29**, 595–604. [8]

Bishop, D. M. (1973): *Group Theory and Chemistry*. Clarendon Press, Oxford. [3, 5]

Bjorken, J. D., Drell, S. D. (1965): *Relativistic Quantum Fields*. McGraw-Hill Book Co., Inc., New York. [5]

Blanco, M. A., Flórez, M., Bermejos, M. (1997): 'Evaluation of the rotation matrices in the basis of real spherical harmonics.' *J. Mol. Struct. (Theochem)* **419**, 19–27. [5]

Blenski, T., Grimaldi, A., Perrot, F. (1997): 'Hartree–Fock statistical approach to atoms and photoabsorption in plasmas.' *Phys. Rev. E* **55**, R4889-R4892. [13]

Blenski, T., Grimaldi, A., Perrot, F. (2000): 'A superconfiguration code based on the local density approximation.' *J. Quant. Spectr. Rad. Transfer* **65**, 91–100. [13]

Bode, G. (1965): 'Die kontinuierliche Absorption von Sternatmosphären in Abhängigkeit von Druck, Temperatur und Elementhäufigkeiten.' Institut für Theoretische Physik und Sternwarte der Universität Kiel report. [1]

Boercker, D. B. (1987): 'Collective effects on Thomson scattering in the solar interior.' *Astrophys. J. Lett.* **316**, L95–L98. [6]

Bogatyrev, K. N. Makarov, V. P. (1994): 'On the vibrational spectrum of a linear molecule.' *Bull. Lebedev Phys. Inst.* Nr. 10, p. 18–22. [5]

Bogatyrev, K. N. Makarov, V. P. (1996): 'Vibration–rotation Hamiltonian of a linear molecule.' *Kratkie Soobshcheniya po Fizike* , No. 9–10, p. 31–36. *Bull. Lebedev Phys. Inst.* Nr. 9, p. 26–31. [5]

Bogatyrev, K. N. Makarov, V. P. (1997a): 'On the theory of the vibration–rotation spectra of linear molecules. I. The molecular Hamiltonian and the "Dirac Rules".' *Optika Spectrosk.* **83**, 733–735. [5]

Bogatyrev, K. N. Makarov, V. P. (1997b): 'On the theory of the vibration–rotation spectra of linear molecules. II. The molecular Hamiltonian.' *Optika Spectrosk.* **83**, 916–920. [5]

Bohm, D. (1951): *Quantum Theory*. Prentice-Hall, Inc., New York. [7]

Bohren, C. F., Huffman, D. R. (1983): *Absorption and Scattering of Light by Small Particles*. John Wiley & Sons, New York, Chichester, Brisbane, Toronto, Singapore. [5]

Boissoles, J., Menous, V., Le Doucen, R., Boulet, C., Robert, D. (1989): 'Collisionally induced population transfer effect infrared absorption spectra. II. Theory of the Ar-broadened ν_3 band of CO_2.' *J. Chem. Phys.* **91**, 2163–2171. [7]

Boissoles, J., Boulet, C., Hartmann, J. M., Perrin, M. Y., Robert, D. (1990): 'Collision-induced population transfer in infrared absorption spectra. III. Temperature dependence of absorption in the Ar-broadened wing of $CO_2\nu_3$ band. *J. Chem. Phys.* **93**, 2217–2221. [7]

Bollé, D. (1981): 'Application of few-body methods to statistical mechanics.' *Nucl. Phys. A* **353**, 377c–389c. [4]

Bond Jr., J. W., Watson, K. M., Welch Jr., J. A. (1965): *Atomic Theory of Gas Dynamics*. Addison-Wesley, Reading, MA. [7]

Bonham, R. A., Lively, M. L. (1984): 'Photon- and electron-impact ionization and ejected-electron angular distributions from molecules including retardation effects: Nonrelativistic theory.' *Phys. Rev. A* **29**, 1224–1235. [5]

Boon, M. H., Seligman, T. H. (1973): 'Canonical transformations applied to the free Landau electron.' *J. Math. Phys.* **14**, 1224–1227. [5]

Borrelli, R., Peluso, A. (2006): 'The vibrational progressions of the N–>V electronic transition of ethylene: A test case for the computation of Franck-Condon factors of highly flexible photoexcited molecules.' *J. Chem. Phys.* **125**, 194308–194308-8. [5]

Borghese, F., Denti, P., Toscano, G., Sindoni, O. I. (1979): 'Electromagnetic scattering by a cluster of spheres.' *Appl. Optics* **18**, 116–120. [5]

Borysow, A. (1991): 'Modeling of collision-induced infrared absorption spectra of H_2-H_2 pairs in the fundamental band at temperatures from 20 to 300 K.' *Icarus* **92**, 273–279. [8]

Borysow, J., Frommhold, L. (1985): 'The infrared and Raman line shapes of pairs of interacting molecules.' In *Phenomena Induced by Intermolecular Interactions*. Ed. G. Birnbaum; Plenum Press, New York, London, p. 67–94. [8]

Borysow, A., Frommhold, L. (1990): 'A new computation of the infrared absorption by H_2 pairs in the fundamental band at temperatures from 600 to 5000 K.' *Astrophys. J.* **348**, L41–L43. [8]

Borysow, A., Frommhold, L., Moraldi, M. (1989): 'Collision-induced infrared spectra of H_2-He pairs involving 0 <–> 1 vibrational transitions and temperatures from 18 to 7000 K.' *Astrophys. J.* **336**, 495–503. [8]

Bosomworth, D. R., Gush, H. P. (1965): 'Collision-induced absorption of compressed gases in the far infrared. II.' *Can. J. Phys.* **43**, 751–769. [13]

Botschwina, P. (1984): 'An ab initio calculation of the frequencies and IR intensities of the stretching vibrations of HN_2^+.' *Chem. Phys. Lett.* **107**, 535–541. [5]

Botschwina, P., Rosmus, P., Reinsch, E.-A. (1983): 'Spectroscopic properties of the hydroxonium ion.' *Chem. Phys. Lett.* **102**, 299–306. [3]

Botschwina, P., Schutz, B., Horn, M., Matuschewski, M. (1995): 'Ab initio calculations of stretching vibrational transitions for the linear molecules HCN, HNC, HCCF, and HC_3N up to high overtones.' *Chem. Phys.* **190**, 345–362. [5]

Boulet, C., Boissoles, J., Robert, D. (1988): 'Collisionally induced population transfer effect in infrared absorption spectra. I. A line-by-line coupling theory from resonances to the far wings.' *J. Chem. Phys.* **89**, 625–634. [7]

Boyle, J. J., Kutzner, M. D. (1998): 'Many-body effects in single photoionization processes.' In *Many-Body Atomic Physics*. Eds. J. J. Boyle and M. S. Pindzola; Cambridge University Press, Cambridge, New York, Melbourne, p. 93–124. [5]

Boynton, F. P., Ludwig, C. B. (1971): 'Total emissivity of hot water vapor: II – Semi-empirical charts deduced from long-path spectral data.' *Int. J. Heat Mass Transfer* **14**, 963–973. [13]
Brandt, W., Lundqvist, S. (1963a): 'Possible new atomic resonances.' *Phys. Lett.* **4**, 47–48. [5]
Brandt, W., Lundqvist, S. (1963b): 'Atomic response function.' *Phys. Rev.* **132**, 2135–2143. [5]
Brandt, W., Lundqvist, S. (1965a): 'Many-electron effects in the dipolar spectra of closed shell atoms.' *Arkiv Fysik* **28**, 399–414. [5]
Brandt, W., Lundqvist, S. (1965b): 'Atomic oscillations in the statistical approximation.' *Phys. Rev.* **139**, A612–A617. [5]
Brandt, W., Lundqvist, S. (1967): 'Collective effects in the photoabsorption cross sections of atoms and molecules.' *J. Quant. Spectr. Rad. Transfer* **7**, 411–421. [5]
Braunstein, M., McKoy, V. (1989): 'Vibrational branching ratios and shape resonant photoionization dynamics in N_2O.' *J. Chem. Phys.* **90**, 1535–1543. [5]
Breene, R. G. (1958): 'Infrared emissivity of NO in high-temperature air.' *J. Chem. Phys.* **29**, 512–516. [7]
Breene Jr., R. G. (1961): *The Shift and Shape of Spectral Lines*. Pergamon Press, New York, Oxford, London, Paris. [7]
Breene Jr., R. G. (1981): *Theories of Spectral Line Shapes.* Wiley, New York. [7]
Breene Jr., R. G., Todd Jr., M. N. (1958): 'Vibrational matrix elements of NO.' *J. Chem. Phys.* **28**, 11–15. [7]
Breit, G. (1926): 'An application of Pauli's method of coordination to atoms having four magnetic parts.' *Phys. Rev.* **28**, 334–340. [7]
Breit, G. (1933): 'Quantum theory of dispersion (continued). Parts VI and VII.' *Rev. Mod. Phys.* **5**, 91–140. [7]
Brink, D. M., Satchler, G. R. (1962): *Angular Momentum*. Clarendon Press, Oxford. [5]
Brion, C. E., Tan, K. H. (1978): 'Partial oscillator strengths for the photoionization of N_2O and CO_2 (20–60 eV).' *Chem. Phys.1978* **34**, 141–151. [5]
Brion, C. E., Tan, K. H. (1981): 'Photoelectron branching ratios and partial oscillator strengths for the photoionization of NO (20–60 eV).' *J. Electron Spectr. Related Phenom.* **23**, 1–11. [5]
Brion, C. E., Thomson, J. P. (1984): 'Compilation of dipole oscillator strengths (cross sections) for the photoabsorption, photoionization and ionic fragmentation of molecules.' *J. Electron Spectr. Related Phenom.* **33**, 301–331. [5]
Brown, R. T. (1972): 'Incoherent-scattering function for atomic carbon.' *Phys. Rev. A* **5**, 2141–2144. [5]
Bruna, P. J., Peyerimhoff, S. D. (1987): 'Excited state potentials.' *Adv. Chem. Phys.* **67**, 1–97. [3]
Bruneau, J., Decoster, A., Desenne, D., Dumont, H., LeBreton, J.-P., Boivineau, M., Perrine, J.-P., Bayle, S., Louis-Jaquet, M., Geindre, J.-P., Chenais-Popovics, C., Gauthier, J.-C. (1991): 'Time-resolved study of hot dense germanium by L-shell absorption spectroscopy.' *Phys. Rev. A* **44**, R832–R835. [13]
Bruning, J. H., Lo, Y. T. (1971a): 'Multiple scattering of EM waves by spheres. Part I. Multipole expansion and ray-optical solutions' *IEEE Trans. Antennas Prop.* **AP-19**, 378–390. [5]
Bruning, J. H., Lo, Y. T. (1971b): 'Multiple scattering of EM waves by spheres. Part II. Umerical and experimental results.' *IEEE Trans. Antennas Prop.* **AP-19**, 391–400. [5]
Brush, S. G., Sahlin, H. L., Teller, E. (1966): 'Monte Carlo study of a one-component plasma. I.' *J. Chem. Phys.* **45**, 2102–2118. [6, 9]
Brussaard, P. J., van de Hulst, H. C. (1962): 'Approximation formulas for nonrelativistic bremsstrahlung and average Gaunt factors for a Maxwellian electron gas.' *Rev. Mod. Phys.* **34**, 507–520. [6]
Brysk, H., Zerby, C. D. (1967): 'Low energy photoelectric cross section calculations.' Union Carbide Corp. Defense and Space Systems Dept. report UCC/DSSD-299, DASA-2023. [3, 5]
Brysk, H., Zerby, C. D. (1968): 'Photoelectric cross sections in the keV range.' *Phys. Rev.* **171**, 292–298. [5]
Brysk, H., Zerby, C. D., Penny, S. K. (1969): 'Bremsstrahlung cross sections at moderate energies.' *Phys. Rev.* **180**, 104–111. [5]

Brysk, H., Campbell, P. M., Hammerling, P. (1975): 'Thermal conduction in laser fusion.' *Plasma Phys.* **17**, 473–484. [9]

Buchler, J. R., Yueh, W. R. (1975): 'Compton scattering opacity.' *Phys. Lett. B* **58**, 463–466. [6]

Buchler, J. R., Yueh, W. R. (1976): 'Compton scattering opacities in a partially degenerate electron plasma at high temperatures.' *Astrophys. J.* **210**, 440–446. [6]

Buckingham, A. D., Orr, B. J., Sichel, J. M. (1970): 'Angular distribution and intensity in molecular photoelectron spectroscopy. I. General theory for diatomic molecules.' *Phil. Trans. Roy. Soc. London, Ser. A* **268**, 147–157. [5]

Buenker, R. J. (1982): 'Implementation of the table CI method: Configurations differing by two in the number of open shells.' *Stud. Phys. Theor. Chem.* **21**, 17–34. [5]

Buenker, R. J., Peyerimhoff, S. D. (1974a): 'Calculations on the electronic spectrum of water.' *Chem. Phys. Lett.* **29**, 253–259. [5]

Buenker, R. J., Peyerimhoff, S. D. (1974b): 'Individualized configuration selection in CI calculations with subsequent energy extrapolation.' *Theor. Chim. Acta* **35**, 33–58. [5]

Buenker, R. J., Peyerimhoff, S. D. (1975): 'Energy extrapolation in CI calculations.' *Theor. Chim. Acta* **39**, 217–228. [5]

Buenker, R. J., Peyerimhoff, S. D. (1983): 'Ab initio calculations close to the full CI level of accuracy and their use for the interpretation of molecular spectra.' In *New Horizons of Quantum Chemistry.* Eds. P.-O. Löwdin and B. Pullman; D. Reidel Publ. Co., Boston, London, p. 183–219. [5]

Buenker, R. J., Peyerimhoff, S. D., Butscher, W. (1978): 'Applicability of the multi-reference double-excitation CI (MRD-CI) method to the calculation of electronic wave functions and comparison with related techniques.' *Mol. Phys.* **35**, 771–791. [5]

Buenker, R. J., Peyerimhoff, S. D., Perić, M. (1979): 'Calculation of vibrational wavefunctions and energies using MRD-CI techniques.' In *Excited States in Quantum Chemistry: Theoretical and Experimental Aspects of the Electronic Structure and Properties of the Excited States in Atoms, Molecules and Solids*. Eds. C. A. Nicolaides and D. R. Beck; D. Reidel Publ. Co., Dordrecht, Boston, London, p. 63–77. [5]

Bunker, P. R. (1979): 'Symmetry in $(H_2)_2$, $(D_2)_2$,.$(HD)_2$ and H_2-D_2 van der Waals complexes.' *Can. J. Phys.* **57**, 2099–2105. [7]

Bunker, P. R. (1985): 'Theoretical predictions of the infrared and microwave spectra of small molecules.' In *Molecular Astrophysics: State of the Art and Future Directions*. Eds. G. H. F. Diercksen, W. F. Huebner, and P. W. Langhoff; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster, p. 491–496. [3]

Bunker, P. R., Jensen, P. (1983): 'A refined potential surface for the $\tilde{X}^3B_1$ state of methylene CH_2.' *J. Chem. Phys.* **79**, 1224–1228. [3]

Bunker, P. R., Langhoff, S. R. (1983): 'Ab initio rotation–vibration transition moments for CH_2 in the X^3B_1 and $\tilde{a}^1A_1$ electronic states.' *J. Mol. Spectr.* **102**, 204–211. [3]

Bunker, P. R., Kraemer, W. P., Spirko, V. (1983a): 'Ab initio rotation-vibration energies of H_3O^+.' *J. Mol. Spectr.* **101**, 180–185. [3]

Bunker, P. R., Sears, T. J., McKellar, A. R. W. (1983b): 'The rotational spectrum of the CD_2 radical.' *J. Chem. Phys.* **79**, 1211–1219. [3]

Burch, D. E. (1981): 'Continuum absorption by H_2O.' Air Force Geophysical Laboratory report AFGL-TR-81-0300. [7]

Burch, D. E. (1985): 'Absorption by H_2O in narrow windows between 3000 and 4200 cm^{-1}.' Air Force Geophys. Lab. report AFGL-TR-850036. [7]

Burch, D. E., Alt, R. L. (1984): 'Continuum absorption by H_2O in 700–1200 cm^{-1} and 2400–2800 cm^{-1} Windows.' Air Force Geophys. Lab. report AFGL-TR-840128 (ADA 1473917 XSP). [7]

Burch, D. E., Singleton, E. B., Williams, D. (1962): 'Absorption line broadening in the infrared.' *Appl. Optics* **1**, 359–363. [7]

Burden, F. R., Wilson R. M. (1972): 'Optimum atomic orbitals for molecular calculations. A review.' *Adv. Phys.* **21**, 825–915. [3]

Burger, H. C., Dorgelo, H. B. (1924): 'Beziehung zwischen inneren Quantenzahlen und Intensitäten von Mehrfachlinien'. *Z. Phys.* **23**, 258–266. [5]

Burgess, A., Seaton, M. J. (1960): 'A general formula for the calculation of atomic photoionization cross sections.' *Mon. Not. Roy. Astron. Soc.* **120**, 121–151. [5]

Burke, P. G. (1965): 'Resonances in electron scattering and photon absorption.' *Adv. Phys.* **14**, 521–567. [5]

Burke, P. G., Seaton, M. J. (1971): 'Numerical solutions of the integro-differential equations of electron – collision theory'. *Meth. Comp. Phys.* **10**, 1–80. [3]

Burke, P. G., Eissner, W. (1983): 'Low-energy electron collisions with complex atoms and ions.' In *Atoms in Astrophysics*. Eds. P. G. Burke, W. Eissner, D. G. Hummer, I. C. Percival; Plenum Press, New York, London, p. 1–54. [3]

Burke, P. G., Hibbert, A., Robb, W. D. (1971): 'Electron scattering by complex atoms.' *J. Phys. B* **4**, 153–161. [3]

Cade, P. E., Huo, W. (1973): 'Hartree–Fock–Roothaan wavefunctions for diatomic molecules: I. First- and second-row hydrides AH, $AH^{\pm}$, AH^{*}.' *Atomic Data Nucl. Data Tables* **12**, 415–466. [3]

Cade, P. E., Huo, W. M. (1975): 'Hartree–Fock–Roothaan wavefunctions for diatomic molecules: III. First-row heteronuclear systems, AB, $AB^{\pm}$, AB^{*}.' *Atomic Data Nucl. Data Tables* **15**, 1–39. [3]

Cade, P. E., Wahl, A. C. (1974): 'Hartree–Fock–Roothaan wavefunctions for diatomic molecules: II. First-row homonuclear systems A_2, $A_2^{\pm}$, A_2^{*}.' *Atomic Data Nucl. Data Tables* **13**, 339–389. [3]

Cade, P. E., Sales, K. D., Wahl, A. C. (1966): 'Electronic structure of diatomic molecules. III. A. Hartree–Fock wavefunctions and energy quantities for N_2 ($X^1\Sigma_g^+$) and N_2^+ ($X^2\Sigma_g^+$, $A^2\Pi_u$, $B^2\Sigma_u^+$) molecular ions.' *J. Chem. Phys.* **44**, 1973–2003. [3]

Caldwell, C. D., Krause, M. O. (1996): 'Photon-atom interactions: Low energy.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 690–700. [5]

Callomon, J. H., Dunn, T. M., Mills, I. M. (1966): 'Rotational analysis of the 2600 angstrom absorption system of benzene.' *Phil. Trans. Roy. Soc. London, Ser. A* **259**, 499–532. [13]

Cambi, R., von Niessen, W. (1983): 'On the photoelectron spectra of HCP and FCP: A Green's function study.' *Chem. Phys. Lett.* **101**, 412–418. [5]

Cameron, A. G. W., Pine, M. R. (1973): 'Numerical models of the primitive solar nebula.' *Icarus* **18**, 377–406. [6]

Camy-Peyret, C., Flaud, J.-M. (1985): 'Vibration-rotation dipole moment operator for asymmetric rotors.' In *Molecular Spectroscopy: Modern Research.* Ed. K. N. Rao; Academic Press, London, Vol. 3, p. 70–110. [5]

Canuto, V. (1970): 'Electrical conductivity and conductive opacity of a relativistic electron gas.' *Astrophys. J.* **159**, 641–652. [9]

Capitelli, M., Colonna, G., Gorse, C., Giordano, D. (1994): 'Survey of methods of calculating high-temperature thermodynamic properties of air species.' European Space Agency report ESA STR-236. [4]

Carbon, D. F. (1974): 'A comparison of the straight-mean, harmonic-mean, and multiple-picket approximations of the line opacities in cool model atmospheres.' *Astrophys. J.* **187**, 135–145. [2]

Carbon, D. F. (1984): 'Line blanketing.' In *Methods of Radiative Transfer.* Ed. W. K. Kalkofen; Cambridge University Press, Cambridge, London, New York, New Rochelle, Melbourne, Sydney, p. 395–426. [7]

Carbon, D. F., Gingerich, O. (1969): 'The grid of model stellar atmospheres from 4000^o to $10{,}000^o$.' In *Theory and Observation of Normal Stellar Atmospheres*. Ed. O. Gingerich; The MIT Press, Cambridge, p. 377–400. [7]

Carlon, H. (1979): 'Do clusters contribute to the IR absorption spectrum of water vapor?' *Infrared Phys.* **19**, 549–558. [7]

Carlson, T. A., Durić, N., Erman, P., Larsson, M. (1979): 'Collisional transfer to the B state in N_2.' *Phys. Scripta* **19**, 25–28. [5]

Carlson, T. A., Keller, P. R., Taylor, J. W., Whitley, T., Grimm, F. A. (1983): 'Angle-resolved photoelectron spectroscopy of N_2O measured as a function of photon energy from 14 to 70 eV.' *J. Chem. Phys.* **79**, 97–106. [5]

Carney, G. D., Porter, R. N. (1976): 'H_3^+: Ab initio calculation of the vibration spectrum.' *J. Chem. Phys.* **65**, 3547–3565. [3]

Carson, T. R. (1971): 'Stellar opacities.' In *Progress in High Temperature Physics and Chemistry*, Vol. 4. Ed. C. A. Rouse; Pergamon Press, Oxford, New York. [1, 9]

Carson, T. R. (1972): 'Stellar opacity.' In *Stellar Evolution*. Eds. H.-Y. Chiu, A. Muriel; MIT Press, Cambridge, MA, London, England. [1]

Carson, T. R. (1976): 'Stellar opacities.' *Ann. Rev. Astron. Astrophys.* **14**, 95–117. [1]

Carson, T. R., Hollingsworth, H. M. (1968): 'A critique of the hydrogenic approximation in the calculation of stellar opacity.' *Mon. Not. Roy. Astron. Soc.* **141**, 77–108. [1, 4]

Carson, T. R., Mayers, D. F., Stibbs, D. W. N. (1968): 'The calculation of stellar radiative opacity.' *Mon. Not. Roy. Astron. Soc.* **140**, 483–536. [1, 4, 5, 12, 13]

Cartwright, D. C., Dunning, T. H. (1975): 'New electronic states of molecular nitrogen (+).' *J. Phys. B* **8**, L100–L104. [3]

Carvajal, M., Arias, J. M., Gómez-Camacho, J. (1999): 'Analytic evaluation of Franck–Condon integrals for anharmonic vibrational wave functions.' *Phys. Rev. A* **59**, 3462–3470. [5, 13]

Case, D. A. (1982): 'Electronic structure calculations using the Xα method.' *Ann. Rev. Phys. Chem.* **33**, 151–171. [3]

Cassisi, S., Potekhin, A. Y., Pietriferni, A., Catelan, M., Salaris, M. (2007): 'Updated electron-conduction opacities: The impact on low-mass stellar models.' *Astrophys. J.* **661**, 1094–1104. [9]

Castor, J. I. (1972): 'Radiative transfer in spherically symmetric flows.' *Astrophys. J.* **178**, 779–792. [2]

Challacombe, M., Schwegler, E., Almlöf, J. (1996): 'Developments in Hartee-fock Theory: Fast methods for computing the Coulomb matrix.' In *Computational Chemistry: Reviews of Current Trends*. Ed., J. Leszczynski, World Scientific, Singapore, New Jersey, London, Hong Kong, Bangalore, Taipei., p. 53–108. [3]

Chandrasekhar, S. (1943): 'Stochastic problems in physics and astronomy.' *Rev. Mod. Phys.* **15**, 1–89. [7]

Chandrasekhar, S. (1960): *Radiative Transfer*. Dover Publications, New York. [2, 5]

Chang, E. S. (1985): 'Radiative lifetime of hydrogenic and quasihydrogenic atoms.' *Phys. Rev. A* **31**, 495–498. [5]

Chang, T.-N. (1998): 'Photoionization dominated by double excitation in two-electron and divalent atoms.' In *Many-Body Atomic Physics*. Eds. J. J. Boyle and M. S. Pindzola; Cambridge University Press, Cambridge, New York, Melbourne, p. 125–149. [5]

Chase Jr., M. W., Davies, C. A., Downey Jr., J. R., Frurip, D. J., McDonald, R. A., Syverud, A. N. (1985): 'JANAF thermodynamical tables,' 3^{rd} ed. *J. Phys. Chem. Ref. Data* **14**, Suppl. 1. [4]

Chase Jr., M. W. (Ed.) (1998): 'NIST-JANAF Thermodynamic Tables, Fourth Edition. *J. Phys. Chem. Ref. Data* Monograph No. 9, Am. Chem. Soc., Washington, DC. [4]

Chau, F.-T., Dyke, J. M., Lee, E. P. F., Wang, D. (1998): 'Franck–Condon analysis of photoelectron and electronic spectra of small molecules.' *J. Electron. Spectr. Rel. Phen.* **97**, 33–47. [5, 7, 13]

Chau, F.-T., Dyke, J. M., Lee, E. P. F., Mok, D. K.-W. (2003): 'Potential energy functions of the $\tilde{X}^2B_1$, $\tilde{A}^2B_2$, $\tilde{B}^2A_1$, and $\tilde{C}^2A_2$ states of Cl_2O^+ and the $\tilde{X}^1A_1$ state of Cl_2O: Franck–Condon simulations of photoelectron bands of Cl_2O which include anharmonicity.' *J. Chem. Phys.* **118**, 4025–4036. [5]

Chen, P. (1994): 'Photoelectron spectroscopy of reactive intermediates.' In *Unimolecular and Biomolecular Ion-Molecule Reaction Dynamics*. Eds. C. Y. Ng, T. Baer, I. Powis, Wiley, New York, p. 371–425. [5]

Chenais-Popovics, C., Merdji, H., Missalla, T., Gilleron, F., Gauthier, J.-C., Blenski, T., Perrot, F., Klapisch, M., Bauche-Arnoult, C., Bauche, J., Bachelier, A., Eidmann, K. (2000): 'Opacity studies of iron in the 15–30 eV temperature range.' *Astrophys. J. Suppl. Ser.* **127**, 275–281. [13]

Child, M. S., Lawton, R. T. (1982): 'Local mode degeneracies in the vibrational spectrum of H_2O.' *Chem. Phys. Lett.* **87**, 217–220. [5]

Chin, C.-W. (1965): 'The opacity due to Compton scattering at relativistic temperatures in a semidegenerate electron gas.' *Astrophys. J.* **142**, 1481–1487. [6]

Christy, R. F. (1966): 'A study of pulsation in RR Lyrae models.' *Astrophys. J.* **144**, 108–179. [11]

Chrysons, M., Kouzov, A. P., Egorova, N. I., Rachet, F. (2008): 'Exact low-order classical moments in collision-induced bands by linear rotors: CO_2–CO_2.' *Phys. Rev. Lett.* **100**, 133007–133010. [8]

Chueh, P. L., Prausnitz, J. M. (1967): 'Vapor-liquid equilibria at high pressures: Calculation of critical temperatures, volumes, and pressures of nonpolar mixtures.' *Am. Inst. Chem. Eng. J.* **13**, 1107–1113. [4]

Čížek, J. (1966): 'On the correlation problem in atomic and molecular systems. Calculation of wavefunction components in Ursell-type expansion using quantum-field theoretical methods.' *J. Chem. Phys.* **45**, 4256–4266. [3]

Clark, T. (1985): *A Handbook of Computational Chemistry: A Practical Guide to Chemical Structure and Energy Calculations.* Wiley, New York. [3]

Clark, R. E. H., Merts, A. L. (1987): 'Quantum defect method applied to oscillator strengths.' *J. Quant. Spectr. Rad. Transfer* **38**, 287–293. [3, 5]

Clementi, E., Raimondi, D. L. (1963): 'Atomic screening constants from SCF functions.' *J. Chem. Phys.* **38**, 2686–2689. [3]

Clementi, E., Raimondi, D. L., Reinhardt, W. P. (1967): 'Atomic screening constants from SCF functions. II. Atoms with 37 to 86 electrons.' *J. Chem. Phys.* **47**, 1300–1307. [3]

Clough, S. A. (1995): 'The water vapor continuum and its role in remote sensing.' *Opt. Remote Sensing Atmosph. (Opt. Soc. Am. Dig. Ser.)* **2**, 76–78. [7]

Clough, S. A., Kneizys, F. X., Davies, R. W. (1989): 'Line shape and the water vapor continuum.' *Atmos. Res.* **23**, 229–241. [7]

Cloutman, L. D. (1973): 'On the accuracy of the Thomas–Fermi atom for opacities.' *Astrophys. J.* **184**, 675–686. [12]

Coester, F., Kümmel, H. (1960): 'Short-range correlations in nuclear wave functions.' *Nucl. Phys.* **17**, 477–485. [3]

Cohen, H. D., Vik, R. C. (1972): 'A Study of Equations of State/Opacity of Ionized Gases.' Systems, Science and Software report 3SR-859-1, DNA 2794F-1. [4]

Cohen, H. D., Parks, D. E., Petschek, A. G. (1971): 'A Study of Equations of State/Opacity of Ionized Gases.' Systems, Science, and Software report 3SR-465, DASA 2597-1. [7]

Cohen, R. S., Spitzer Jr., L., Routly, P. McR. (1950): 'The electrical conductivity of an ionized gas.' *Phys. Rev.* **80**, 230–238. [9]

Coker, D. F., Miller, R. E., Watts, R. O. (1985): 'The infrared predissociation spectra of water clusters.' *J. Chem. Phys.* **82**, 3554–3562. [5]

Colgan, J., Fontes, C. J., Abdallah, Jr., J. (2006): 'Collisional radiative studies of carbon plasmas.' *High Energy Dens. Phys.* **2**, 90–96. [14]

Collins, L. A., Schneider, B. (1984): 'Molecular photoionization in the linear algebraic approach: H_2, N_2, NO, and CO_2.' *Phys. Rev. A* **29**, 1695–1708. [5]

Colvin, M. E., Raine, G. P., Schaefer III, H. F. (1983): 'Infrared intensities of H_3O^+, H_2DO^+, HD_2O^+, and D_3O^+.' *J. Chem. Phys.* **79**, 1551–1552. [3]

Condon, E. U. (1928): 'Nuclear motions associated with electron transitions in diatomic molecules.' *Phys. Rev.* **32**, 858–872. [6]

Condon, E. U., Shortley, G. H. (1953): *The Theory of Atomic Spectra*. University Press, Cambridge, 1935 (reprinted with corrections 1953). [3, 5, 7]

Condon, E. U., Odabaşı, H. (1980): *Atomic Structure*. Cambridge University Press, Cambridge, London, New York, New Rochelle, Melbourne, Sydney. [3]

Cooley, J. W. (1961): 'An improved eigenvalue corrector formula for solving the Schrödinger equation for central fields.' *Math. Comp.* **15**, 363–374. [3]
Coolidge, A. S., James, H. M., Present, R. D. (1936): 'A study of the Franck–Condon principle.' *J. Chem. Phys.* **4**, 193–211. [6]
Coon, J. B., DeWames, R. E., Loyd, C. M. (1962): 'The Franck–Condon principle and the structures of excited electronic states of molecules.' *J. Mol. Spectr.* **8**, 285–299. [5]
Cooper, D. M., Langhoff, S. R. (1981): 'Theoretical study of selected singlet and triplet states of the CO molecule.' *J. Chem. Phys.* **74**, 1200–1210. [10]
Cooper, J. W. (1964): 'Interaction of maxima in the absorption of soft x rays.' *Phys. Rev. Lett.* **13**, 762–764. [5]
Cooper, J., Zare, R. N. (1968): 'Angular distribution of photoelectrons.' *J. Chem. Phys.* **48**, 942–943. [5]
Corben, H. C., Schwinger, J. (1940): 'The electromagnetic properties of mesotrons.' *Phys. Rev.* **58**, 953–968. [5]
Corliss, C. H., Bozman, W. R. (1962): *Experimental Transition Probabilities for Spectral Lines of Seventy Elements*. National Bureau of Standards Monograph 53. [5]
Costescu, A., Vrejoiu, C., Bogatu, N. (1981): 'On the average bremsstrahlung spectral distribution and energy loss in fully ionized plasmas.' *Rev. Roum. Phys.* **26**, 281–301. [5]
Courtin, R. (1988): 'Pressure-induced absorption coefficients for radiative transfer calculations in Titan's atmosphere.' *Icarus* **75**, 245–254. [8, 13]
Cousin, C., Le Doucen, R., Boulet, C. (1986): 'Line coupling in the temperature and frequency dependencies of absorption in the microwindows of the 4.3 μm CO_2 band.' *J. Quant. Spectr. Rad. Transfer* **36**, 521–538. [7]
Cowan, R. D. (1967): 'Atomic self-consistent-field calculations using statistical approximations for exchange and correlation.' *Phys. Rev.* **163**, 54–61. [3]
Cowan, R. D. (1968): 'Theoretical calculation of atomic spectra using digital computers.' *J. Opt. Soc. Am.* **58**, 808–818. [3]
Cowan, R. D. (1981): *The Theory of Atomic Structure and Spectra*. University of California Press, Berkeley, Los Angeles, London. [3, 4, 5, 7]
Cowan, R. D., Andrew, K. L. (1965): 'Coupling considerations in two-electron spectra.' *J. Opt. Soc. Am.* **55**, 502–516. [3]
Cowan, R. D., Ashkin, J. (1957): 'Extension of the Thomas–Fermi–Dirac statistical theory of the atom to finite temperatures.' *Phys. Rev.* **105**, 144–157. [4]
Cowan, R. D., Kirkwood, J. G. (1958a): 'Quantum statistical theory of plasmas and liquid metals.' *J. Chem. Phys.* **29**, 264–271. [4]
Cowan, R. D., Kirkwood, J. G. (1958b): 'Quantum statistical theory of electron correlation.' *Phys. Rev.* **111**, 1460–1466. [4]
Cowley, C. R. (1970): *Theory of Stellar Spectra*. Gordon & Breach Science Publishers, New York, London, Paris. [1]
Cox, A. N. (1965): 'Stellar absorption coefficients and opacities.' In *Stars and Stellar Systems, Vol. 8: Stellar Structure*, p. 195–268. Eds. L. H. Aller, D. B. McLaughlin; The University of Chicago Press, Chicago. [1, 4, 9, 11]
Cox, A. N. (2000): *Allen's Astrophysical Quantities*. 4^{th} edition, Springer, AIP Press, New York, NY. [7]
Cox, A. N., Stewart, J. N. (1965): 'Radiative and conductive opacities for eleven astrophysical mixtures.' *Astrophys. J. Suppl. Ser.* **11**, 22–46. [1, 9, 12]
Cox, A. N., Stewart, J. N., Eilers, D. D. (1965): 'Effects of bound-bound absorption on stellar opacities.' *Atrophys. J. Suppl. Ser.* **11**, 1–21. [1]
Cox, J. P., Giuli, R. T. (1968): *Principles of Stellar Structure*. Gordon Beach, New York. [6]
Craig, D. P., Thirunamachandran, T. (1984): *Molecular Quantum Electrodynamics: An Introduction to Radiation-Molecule Interactions*. Academic Press, New York, Orlando, San Diego. [3, 5]
Crawford Jr., B. L., Dinsmore, H. L. (1950): 'Vibrational intensities. I. Theory of diatomic infra-red bands.' *J. Chem. Phys.* **18**, 983–987; **18**, 1682–1683. [5, 7]

Crecely, R. W., Wilson, D. J. (1964): 'Thermodynamic functions of Morse oscillators.' *J. Chem. Phys.* **41**, 1564–1567. [4]

Crees, M. A., Seaton, M. J., Wilson, P. M. H. (1978): 'Impact, a program for the solution of the coupled integro-differential equations of electron – atom collision theory.' *Comp. Phys. Comm.* **15**, 23–83. [3]

Cromer, D. T. (1969): 'Compton scattering factors for aspherical free atoms.' *J. Chem. Phys.* **50**, 4857–4859. [5]

Cromer, D. T., Mann, J. B. (1967): 'Compton scattering factors for spherically symmetric free atoms.' *J. Chem. Phys.* **47**, 1892–1893. [5]

Cromer, D. T., Waber, J. T. (1964): 'Scattering Factors Computed from Relativistic Dirac–Slater Wave Functions.' Los Alamos Scientific Laboratory report LA-3056. [5]

Cross, P. C., Hainer, R. M., King, G. W. (1944): 'The asymmetric rotor. II. Calculation of dipole intensities and line classification.' *J. Chem. Phys.* **12**, 210–243. [5]

Crowley, B. J. B., Harris, J. W. (2001): 'Modelling of plasmas in an average-atom local density approximation: The CASSANDRA code.' *J. Quant. Spectr. Rad. Transfer* **71**, 257–272. [13]

Cruzan, O. R. (1962): 'Translational addition theorems for spherical vector wave functions.' *Quart. Appl. Math.* **20**, 33–40. [5]

Csanak, G., Kilcrease D. (1993): 'Photo absorption in hot dense plasmas - the average atom (AA), the spherical cell (SC), and the random phase approximation.' *J. Quant. Spectr. Rad. Transfer* **58**, 537–551. [4]

Cunio, B. E., Jansson, R. E. W. (1968): 'The electronic transition moment of the N_2 first positive system (N_2 1PG).' *J. Quant. Spectr. Rad. Transfer* **8**, 1763–1771. [5]

Curtis, A. R. (1952): 'A statistical model fro water-vapour absorption.' *Quart. J. Roy. Met. Soc.* **78**, 638–640. [7]

Curtis, L. J. (1996): 'Precision oscillator strength and lifetime measurements.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 206–212. [5]

Däppen, W., Anderson, L., Mihalas, D. (1987): 'Statistical mechanics of partially ionized stellar plasmas: The Planck–Larkin partition function, polarization shifts, and simulations of optical spectra.' *Astrophys. J.* **319**, 195–206. [4]

Däppen, W., Mihalas, D., Hummer, D. G., Weibel Mihalas, B. (1988): 'The equation of state for stellar enveloopes. III. Thermodynamic quantities.' *Astrophys. J.* **332**, 261–270. [4]

Dagdeviren, N. R., Koonin, S. E. (1987): 'Effect of ion correlations on free–free opacities.' *Astrophys. J.* **319**, 192–194. [6]

Dagg, I. R., Anderson, A., Yan, S., Smith, W., Read, L. A. A. (1986a): 'Collision-induced absorption in nitrogen at low temperatures.' *Can. J. Phys.* **63**, 625–631. [13]

Dagg, I. R., Anderson, A., Yan, S., Smith, W., Joslin, G. G., Read, L. A. A. (1986b): 'Collision-induced absorption in gaseous mixtures of nitrogen and methane.' *Can. J. Phys.* **64**, 1467–1474. [13]

Danese, J. B., Connolly, J. W. D. (1974): 'Calculation of the total energy in the multiple scattering-$X\alpha$ method. I. General theory.' *J. Chem. Phys.* **61**, 3063–3080. [3]

Da Silva, L. B., MacGowen, B. J., Kania, D. R., Hammel, B. A., Back, C. A., Hsieh, E., Doyas, R., Iglesias, C. A., Rogers, F. J., Lee, R. W. (1992): 'Absorption measurements demonstrating the importance of $\Delta n = 0$ transitions in the opacity of iron.' *Phys. Rev. Lett.* **69**, 438–441. [13]

Davenport, J. W. (1977): 'Multiple scattering theory of photoemission.' *Int. J. Quantum Chem. Symp.* **11**, 89–96. [5]

Davidson, E. R., Feller, D. (1986): 'Basis set selection for molecular calculations.' *Chem. Rev.* **86**, 681–696. [3]

Davidson, S. J., Foster, J. M., Smith, C. C., Warburton, K. A., Ross, S. J. (1989): 'Investigation of the opacity of hot, dense Al in the region of its K-edge.' *Appl. Phys. Lett.* **52**, 847–849. [13]

Davies, R. W., Tipping, R. H., Clough, S. A. (1982): 'Dipole auto-correlation function for molecular pressure broadening : A quantum theory which satisfies the fluctuation-dissipation theorem.' *Phys. Rev. A* **26**, 3378–3394. [7]

Davis, J. (1974): 'Effective Gaunt factors for electron impact excitation of multiply charged nitrogen and oxygen ions.' *J. Quant. Spectr. Rad. Transfer* **14**, 549–554. [7]

Davis, J., Kepple, P. C., Blaha, M. (1975): 'Distorted wave calculations for multiply charged nitrogen and oxygen.' *J. Quant. Spectr. Rad. Transfer* **15**, 1145–1148. [7]

Davydkin, V. A., Zon, B. A. (1981): 'Radiation and polarization characteristics of Rydberg atomic states.' *Optics Spectrosc.* **51** 13–15. [5]

Dawson, J. M. (1964): 'On the production of plasma by giant pulse lasers.' *Phys. Fluids* **7**, 981–987. [6]

Dawson, J., Oberman, C. (1962): 'High-frequency conductivity and the emission and absorption coefficients of a fully ionized plasma.' *Phys. Fluids* **5**, 517–524. [6, 9]

Dawson, J., Oberman, C. (1963): 'Effect of ion correlations on high-frequency plasma conductivity.' *Phys. Fluids* **6**, 394–397. [6, 9]

Day, K. L. (1979): 'Mid-infrared optical properties of vapor-condensed magnesium silicates.' *Astrophys. J.* **234**, 158–161. [6]

Dehmer, J. L., Dill, D. (1979): 'The continuum multiple-scattering approach to electron–molecule scattering and molecular photoionization.' In *Electron–Molecule and Photon–Molecule Collisions.* Eds. T. Rescigno, V. McKoy, and B. Schneider; Plenum Press, New York, London, p. 225–263. [5]

Dehmer, J. L., Parr, A. C., Southworth, S. H., Holland, D. M. P. (1983a): 'Triply differential photoelectron studies of molecular photoionization.' In *13*th *Int. Conf. on the Physics of Electronic and Atomic Collisions*, Berlin. North-Holland, Amsterdam, p. 341–408. [5]

Dehmer, J. L., Dill, D., Parr, A. C. (1983b): 'Photoionization dynamics of small molecules.' In *Photophysics and Photochemistry in the Vacuum Ultraviolet*. Eds. S. McGlynn, G. Finley, and R. Huebner; D. Reidel Publishing Co., Dordrecht, p. 341–408. [5]

Dehmer, J. L., Parr, A. C., Southworth, S. H. (1987): 'Resonances in molecular photoionization.' In *Handbook on Synchrotron Radiation.* Vol. 2, Ed. G. V. Marr; North-Holland, Amsterdam, Oxford, New York, Tokyo, p. 241–353. [5]

Deirmendjian, D. (1969): *Electromagnetic Scattering on Spherical Polydispersions*. American Elsevier Publishing Co., Inc., New York. [5]

Dennison, D. M. (1926): 'The rotation of molecules.' *Phys. Rev.* **28**, 318–333. [5]

Dennison, D. M. (1940): 'Infra-red spectra of polyatomic molecules. Part II.' *Rev. Mod. Phys.* **12**, 175–214. [5]

Desclaux, J. P. (1983a): 'Numerical Dirac–Fock calculations for atoms.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 115–144. [3]

Desclaux, J. P. (1983b): 'Dirac–Fock one-centre expansion method.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 213–226. [3]

Detrich, J. H., Roothaan, C. C. J. (1981): 'Calculation of relativistic effects in atoms and molecules from the Schrödinger wave function.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 169–182. [3]

DeWitt, H. E., Rogers, F. J. (1972): 'Quantum statistical mechanics of dense partially ionized hydrogen.' *Phys. Earth Planet. Interiors* **6**, 51–59. [4]

de Zotti, G. (1975): 'Free-free opacity of dense stellar matter.' *Astrophys. Space Sci.* **33**, 359–367. [6]

Diercksen, G. H. F., Sadlej, A. J. (1985): 'Finite-field many-body perturbation theory. VII. A complete fourth-order MBPT study of multipole moments of the CO molecule.' *Chem. Phys.* **96**, 17–41. [5]

Diercksen, G. H. F., Kraemer, W. P., Rescigno, T. N., Bender, C. F., McKoy, B. V., Langhoff, S. R., Langhoff, W. P. (1982): 'Theoretical studies of photoexcitation and ionization in H_2O.' *J. Chem. Phys.* **76**, 1043–1057. [5]

Diercksen, G. H. F., Grüner, N. E., Steuerwald, J. (1983a): 'Computers and computations.' In *Methods in Computational Molecular Physics*. Eds. G. H. F. Diercksen and S. Wilson; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster, Vol. **113**, p. 335–350. [3]

Diercksen, G. H. F., Roos, B. O., Sadlej, A. (1983b): 'Electron correlation and properties of many-electron systems.' *Int. J. Quantum Chem. Symp.* **17**, 265–288. [3]

Diesendorf, M., Ninham, B. W. (1968): 'Quantum corrections to the pair distribution function of a classical plasma.' *J. Math. Phys.* **9**, 745–752. [6]

Diesendorf, M., Ninham, B. W. (1969): 'The effect of quantum correlations on electron-scattering opacities.' *Astrophys. J.* **156**, 1069–1073. [6]

Dill, D., Dehmer, J. L. (1974): 'Electron–molecule scattering and molecular photoionization using the multiple-scattering method.' *J. Chem. Phys.* **61**, 692–699. [5]

Dill, D., Starace, A. F., Manson, S. T. (1975): 'Effects of anisotropic electron–ion interactions in atomic photoelectron angular distribution.' *Phys. Rev. A* **11**, 1596–1606. [5]

Dingle, R. B. (1957): 'The Fermi–Dirac integrals: $\mathcal{F}_{\wp}(\eta) = (\wp!)^{-1}\int_0^{\infty} \varepsilon^{\wp}(e^{\varepsilon-\eta}+1)^{-1} d\varepsilon.'$ *Appl. Sci. Res.* **6B**, 225–239. [9, App. C]

Dirac, P. A. M. (1927a): 'The quantum theory of emission and absorption of radiation.' *Proc. Roy. Soc. (London), Ser. A* **114**, 243–265. [5]

Dirac, P. A. M. (1927b): 'The quantum theory of dispersion.' *Proc. Roy. Soc. (London), Ser. A* **114**, 710–728. [7]

Dirac, P. A. M. (1930): 'Note on exchange phenomena in the Thomas atom.' *Proc. Cambridge Phil. Soc.* **26**, 376–385. [3]

Doggett, J. A., Spencer, L. V. (1956): 'Elastic scattering of electrons and positrons by point nuclei.' *Phys. Rev.* **103**, 1597–1601. [9]

Dogliani, H. O., Bailey, W. F. (1969): 'A relativistic correction to the Thomas–Kuhn sum rule.' *J. Quant. Spectr. Rad. Transfer* **9**, 1643–1645. [6]

Doktorov, E. V., Malkin, I. A., Man'ko, V. I. (1975): 'Dynamical symmetry of vibronic transitions in polyatomic molecules and the Franck–Condon principle.' *J. Mol. Spectr.* **56**, 1–20. [5, 7]

Doktorov, E. V., Malkin, I. A., Man'ko, V. I. (1976): 'Dynamical symmetry of vibronic transitions with degenerate vibrations and the Franck–Condon factors.' *J. Phys. B* **9**, 507–514. [5]

Doktorov, E. V., Malkin, I. A., Man'ko, V. I. (1977a): 'The Franck–Condon principle and sum rules for vibronic transitions in polyatomic molecules.' *Chem. Phys. Lett.* **46**, 183–187. [7]

Doktorov, E. V., Malkin, I. A., Man'ko, V. I. (1977b): 'Dynamical symmetry of vibronic transitions in polyatomic molecules and the Franck-Condon principle.' *J. Mol. Spectr.* **64**, 302–326. [5, 7]

Domcke, W., Cederbaum, L. S., Köppel, H., von Niessen, W. (1977): 'A comparison of different approaches to the calculation of F–C factors for polyatomic molecules.' *Molec. Phys.* **34**, 1759–1770. [5]

Domoto, G. A. (1974): 'Frequency integration for radiative transfer problems involving homogeneous non-gray gases: The inverse transmission function.' *J. Quant. Spectr. Rad. Transfer* **14**, 935–42. [7]

Dorschner, J. (1970): 'Theoretische Untersuchung über den interstellaren Staub. II. Optische Eigenschaften kugelförmiger Staubteilchen aus meteoritischen Silikaten und aus schmutzigem Eis.' *Astron. Nachrichten* **292**, 71–78. [5]

Dragalov, V. V., Novikov, V. G. (1988): 'Distribution of spectral lines in plasma with respect to the fluctuations of the filling number.' *Teplofizika Vysokikh Temperatur* **25**, 1057–1061 (*High Temp.* **25**, 762–766). [7]

Dragalov, V. V., Novikov, V. G. (1989a): 'Average-atom calculation of the energy of dipole transitions in highly ionized plasmas of heavy elements.' *Fiz. Plazmy* **15**, 493–495 (*Sov. J. Plasma Phys.* **15**, 288–289). [7]

Dragalov, V. V., Novikov, V. G. (1989b): 'Approximate ion-configuration correction in calculating photoionization cross sections for a dense hot plasma.' *Teplofizika Vysokikh Temperatur* **27**, 214–219 (*High Temp.* **27**, 161–165). [6]

Dragalov, V. V., Nikiforov, A. F., Novikov, V. G., Uvarov, V. B. (1990): 'Statistical method for calculating the absorption of photons in dense high-temperature plasmas.' *Fiz. Plazmy* **16**, 77–85 (*Sov. J. Plasma Phys.* **16**, 44–49). [7]

Dufresne, J. I., Fournier, R., Grandpeix, J. Y. (1999): 'Inverse Gaussian k-distributions.' *J. Quant. Spectr. Rad. Transfer* **61**, 433–441. [7]

Dufty, J. W., Boerker, D. B., Iglesias, C. A. (1985): 'Electric field distributions in strongly coupled plasmas.' *Phys. Rev. A* **31**, 1681–1686. [7]

Dunham, J. L. (1930): 'Intensities of vibration-rotation bands with special reference to those of HCl.' *Phys. Rev.* **85**, 1347–1354. [7]

Dunham, J. L. (1932): 'The Wentzel-Brillouin-Kramers method of solving the wave equation.' *Phys. Rev.* **41**, 713–720. [3]

Dunning Jr., T. H., McKoy, V. (1968): 'Nonempirical calculations on excited states: The formaldehyde molecule.' *J. Chem. Phys.* **48**, 5263–5270. [3]

Dunning Jr., T. H., Hunt, W. J., Goddard III, W. A. (1969): 'The theoretical description of the $(\pi\pi^*)$ excited states of ethylene.' *Chem. Phys. Lett.* **4**, 147–150. [3]

Dunning Jr., T. H., Cartwright, D. C., Hunt, W. J., Hay, P. J., Bobrowicz, F. W. (1976): 'Generalized valence bond calculations in the ground state $(X^1\Sigma_g^+)$ of nitrogen.' *J. Chem. Phys.* **64**, 4755–4766. [3]

Dupuis, M., Wendoloski, J. J. (1984): 'Systematic GVB study of harmonic vibrational frequencies and dipole moment derivatives; the vinyl radical C_2H_3 and other simple molecules.' *J. Chem. Phys.* **80**, 5696–5702. [5]

Duschinsky, F. (1937): 'Zur Deutung der Elektronenspektren mehratomiger Moleküle. I. Über das Franck–Condon Prinzip.' *Acta Physicochim. URSS* **7**, 551–566. [5]

Dykstra, G. E. (1984): *Advanced Theories and Computational Approaches to the Electronic Structure of Molecules.* D. Reidel Publ. Co., Dordrecht, Boston, Lancaster. [3]

Dykstra, C. E., Schaefer III, H. F. (1976a): 'A theory of self-consistent electron pairs. Computational methods and preliminary applications.' *J. Chem. Phys.* **65**, 2740–2750. [5]

Dykstra, C. E., Schaefer III, H. F. (1976b): 'Electron correlation in small metal clusters. Application of a theory of self-consistent electron pairs to the Be_4 system.' *J. Chem. Phys.* **65**, 5141–5146. [5]

Dykstra, C. E., Schaefer III, H. F. (1984): 'Computer technology in quantum chemistry.' In *Advanced Theories and Computational Approaches to the Electronic Structure of Molecules*. Ed. C. E. Dykstra; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster. p. 197–202. [3]

Dyson, F. J. (1958): 'Note on maximum opacity.' General Atomic report GAMD-469. [11]

Ebeling, W., Kraeft, W. D., Kremp, D. (1977): *Theory of Bound States and Ionization Equilibrium in Plasmas and Solids.* Akademie Verlag, Berlin. [4]

Eby, P. B., Sung, C. C. (1986): 'Comparison of exact and approximate formulas for the Mott correction to energy loss of relativistic heavy ions.' *Phys. Rev. A* **33**, 3767–3773. [9]

Eckart, C. (1935): 'Some studies concerning rotating axes and polyatomic molecules.' *Phys. Rev.* **47**, 552–558. [3, 5]

Ecker, G., Müller, K. G. (1958): 'Plasmapolarisation und Trägerwechselwirkung.' *Z. Phys.* **153**, 317–330. [7]

Ederer, D. L. (1964): 'Photoionization of the 4d electrons in xenon.' *Phys. Rev. Lett.* **13**, 760–762. [5]

Edmonds, A. R. (1957): *Angular Momentum in Quantum Mechanics.* Princeton U. Press, Princeton, N.J. [5]

Edmonds, A. R., Picart, J., Tran Minh, N., Pullen, R. (1979): 'Tables for the computation of radial integrals in the Coulomb approximation.' *J. Phys.* **B 12**, 2781–2787. [5]

Edwards, D. K., Flornes, B. J., Glassen, L. K., Sun, W. (1965): 'Correlation of absorption by water vapor at temperatures from 300 to 1100 K.' *Appl. Optics* **4**, 715–721. [13]

Eissner, W. (1972): 'Computer methods and packages in electron – atom collisions (II). In *The Physics of Electronic and Atomic Collisions*. Eds. T. R. Grovers and F. J. de Heer. North-Holland Publ. Co., Amsterdam, London, p. 460–478. [3]

Eissner, W., Seaton, M. J. (1972): 'Computer programs for the calculation of electron – atom collision cross sections. I. General formulation.' *J. Phys. B* **5**, 2187–2198. [3]

Eissner, W., Jones, M., Nussbaumer, H. (1974): 'Techniques for the calculation of atomic structures and radiative data including relativistic corrections.' *Comp. Phys. Comm.* **8** 270–306. [3]

Elliott, P., Furche, F., Burke, K. (2009): 'Excited states from time-dependent density functional theory.' In *Rev. Comp. Chem.* **26**, 91–165. Eds. K. B. Lipkowitz, T. R. Cundari; John Wiley Sons. [3]

Elsasser, W. M. (1938): 'Mean absorption and equivalent absorption coefficient of a band spectrum.' *Phys. Rev.* **54**, 126–129. [7, 11]

Elsasser, W. M. (1942): 'Heat transfer by IR radiation in the atmosphere.' *Harvard Meteorological Studies No. 6*, Milton, MA, and Oxford U. Press, London. [7]

Elwert, G. (1939): 'Intensity and polarization in the continuous x-ray spectrum.' *Ann. Phys.* **34**, 178–208. [6]

Elwert, G. (1954): 'Die weiche Röntgenstrahlung der ungestörten Sonnenkorona.' *Z. Naturforsch.* **9a**, 637–653. [6]

Elwert, G., Haug, E. (1969): 'Calculation of bremsstrahlung cross sections with Sommerfeld-Maue eigenfunctions.' *Phys. Rev.* **183**, 90–105. [5]

Engel, E., Vosco, S. H. (1990): 'Wave-vector dependence of the exchange contribution to the electron-gas response functions: An analytic derivation.' *Phys. Rev. B* **42**, 4940–4953. [3]

Engel, E., Vosco, S. H. (1993): 'Exact exchange-only potentials and the virial relation as microscopic criteria for generalized gradient approximations.' *Phys. Rev. B* **47**, 13164–13174. [3]

Engel, V., Schinke, R., Staemmler, V. (1986): 'An ab initio calculation of the absorption cross section of water in the first absorption continuum.' *Chem. Phys. Lett.* **130**, 413–418. [5]

Engel, V., Staemmler, V., Vander Wal, R. L., Crim, F. F., Sension, R. J., Hudson, B., Andresen, P., Hennig, S., Weide, K., Schinke, R. (1992): 'Photodissociation of water in the first absorption band: A prototype for dissociation on a repulsive potential energy surface.' *J. Phys. Chem.* **96**, 3201–3213. [5]

Engelhardt, A. G., Phelps, A. V., Risk, C. G. (1964): 'Determination of momentum transfer and inelastic collision cross sections for electrons in nitrogen using transport coefficients.' *Phys. Rev.* **135**, A1566–A1574. [6]

Engler, E. M., Andose, J. D., Schleyer, P. V. R. (1973): 'Critical evaluation of molecular mechanics.' *J. Am. Chem. Soc.* **95**, 8005–8025. [3]

Enskog, D. (1922): 'Kinetic theory of heat conductivity, viscosity and diffusion in certain condensed gases and liquids.' *Kungl. Svenska Vetenskap. Handl.* **63**, 1–44. [9]

Erdelyi, A. (1953): *Higher Transcendental Functions*, Vol. 2. McGraw-Hill, New York, Toronto, London. [5]

Eriksson, G. (1971): 'Thermodynamic studies of high temperature equilibria. III. SOLGAS, a computer program for calculating the composition and heat condition of an equilibrium mixture.' *Acta Chem. Scandinavica* **25**, 2651–2658. [4]

Eriksson, G. (1975): 'Thermodynamic studies of high temperature equilibria. XII. SOLGASMIX, a computer program for calculation of equilibrium compositions in multiphase systems.' *Chem. Scripta* **8**, 100–103. [4]

Eriksson, G., Rosén, E. (1973): 'Thermodynamic studies of high temperature equilibria. VIII. General equations for the calculation of equilibria in multiphase systems.' *Chem. Scripta* **4**, 193–194. [4]

Ermler, W. C., Rosenberg, B. J., Shavitt, I. (1985): 'Ab-initio SCF and CI studies on the ground state of the water molecule. III. Vibrational analysis of potential energy and property surfaces.' In *Comparison of Ab Initio Calculations with Experiment: State of the Art.* Ed. R. Bartlett; D. Reidel Publ. Co., Dordrecht, p. 171–216. [5]

Eschrig, H. (1989): *Optimized LCAO method and the electronic structure of extended systems.* Springer-Verlag, Berlin. [3]

Evans, J. S., Schexnayder Jr., C. J. (1961): 'An investigation of the effect of high temperature on the Schumann-Runge ultraviolet absorption continuum of oxygen.' National Aeronautic and Space Administration report NASA TR R-92. [6]

Ewart, G. M., Guyer, R. A., Greenstein, G. (1975): 'Electrical conductivity and magnetic field decay in neutron stars.' *Astrophys. J.* **202**, 238–247. [9]

Eyler, E. E., Pipkin, F. M. (1983): 'Lifetime measurements of the $B^3\Pi_g$ state of N_2 using laser excitation.' *J. Chem. Phys.* **79**, 3654–3659. [5]

Faddeyeva, V. N., Terentev, V. M. (1961): *Tables of the Probability Integral for Complex Argument*. Pergamon Press, New York. [7]

Fano, U. (1961): 'Effects of configuration interaction on intensities and phase shifts.' *Phys. Rev.* **124**, 1866–1878. [5]

Fano, U., Cooper, J. W. (1965): 'Line profiles in the far-UV absorption spectra of the rare gases.' *Phys. Rev.* **137**, A1364–A1379. [5]

Fano, U., Cooper, J. W. (1968): 'Spectral distribution of atomic oscillator strengths.' *Rev. Mod. Phys.* **40**, 441–507. [1, 5]

Fermi, E. (1949): *Nuclear Physics*. The University of Chicago Press. [5, 7]

Fermi, E., Amaldi, E. (1934): 'Le orbite ∞ s degli elementi.' *Mem. Reale Accad. Italia* **6**, 119–149. [3]

Ferriso, C. C., Ludwig, C. B. (1964): 'Spectral emissivities and integrated intensities of the 2.7 micron H_2O band between 530 and 2200 K.' *J. Quant. Spectr. Rad. Transfer* **4**, 215–227. [13]

Ferriso, C. C., Ludwig, C. B., Thomson, A. L. (1966): 'Empirically determined infrared absorption coefficients of H_2O from 300 to 3000 K.' *J. Quant. Spectr. Rad. Transfer* **6**, 241–275. [13]

Feynman, R. P., Metropolis, N., Teller, E. (1949): 'Equations of state of elements based on the generalized Fermi–Thomas theory.' *Phys. Rev.* **75**, 1561–1573. [4]

Finn, G. D., Mugglestone, D. (1965): 'Tables of the line broadening function $H(a, v)$.' *Mon. Not. Roy. Astron. Soc.* **129**, 221–235. [7]

Fiolhais, C., Nogueira, F., Marques, M. (Eds.) (2003): *A Primer in Density Functional Theory.* Lecture Notes in Physics, **620**, Springer-Verlag, New York, NY. [3]

Fischer, C. F. (1996): 'Atomic structure: Multiconfiguration Hartree–Fock theories.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 243–257. [3]

Fischer, J. (1931a): 'Beiträge zur Theorie der Absorption von Röntgenstrahlen.' *Ann. Physik* **8**, 821–850. [5]

Fischer, J. (1931b): 'Über die retardierten Matrixelemente in der Theorie der Streuung und Absorption von Röntgenstrahlen.' *Ann. Physik* **11**, 489–520. [5]

Flaud, J.-M., Camy-Peyret, C., Toth, R. A. (1981): *Parametres des raies de la vapeur d'eau des micro-ondes a l'infrarouge moyen (Atlas des positions et intensites des raies de $H_2^{16}O$, $H_2^{17}O$ et $H_2^{18}O$ entre 0 et 4350 cm^{-1})*. Pergamon Press, Oxford, New York, Toronto, Sydney, Paris, Frankfurt. [7]

Flowers, E., Itoh, N. (1976): 'Transport properties of dense matter.' Astrophys. J. **206**, 218–242. [9]

Flowers, E., Itoh, N. (1981): 'Transport properties of dense matter. III Analytic formulae for thermal conductivity.' Astrophys. J. **250**, 750–752. [9]

Ford, A. L., Docken, K. K., Dalgarno, A. (1975): 'The photoionization and dissociative ionization of H_2, HD, and D_2.' *Astrophys. J.* **195**, 819–824. [5]

Foster, J. M., Hoarty, D. J., Smith, C. C., Rosen, P. A., Davidson, S. J., Rose, S. J., Perry, T. S., Serduke, F. J. D. (1991): 'L-shell absorption spectrum of an open-M-shell germanium plasma: Comparison of experimental data with a detailed configuration-accounting calculation.' *Phys. Rev. Lett.* **67**, 3255–3258. [13]

Fox, J. L. (1991): 'Cross sections and reaction rates of relevance to aeronomy.' *Revs. Geophys.* **29**, Suppl. 2, 1110–1131. [5]

Fox, K., Ozier, I. (1971): 'The importance of methane to pressure-induced absorption in the atmospheres of the outer planets.' *Astrophys. J. Lett.* **166**, L95–L100. [8, 13]

Fraga, S., Saxena, K. M. S., Karwowski, J. (1979): *Atomic Energy Levels: Data for Parametric Calculations.* Elsevier Scientific Publ. Co.; Amsterdam, New York. [3, 4]

Frank-Kamenetski, D. A. (1962): 'Macroscopic theory of radiant energy transport processes.' Translated by M. J. Nowak. In *Physical Processes in Stellar Interiors,* Chap. 5. (1959): Jerusalem, Israel Program for Scientific Translations (Office of Tech. Services, US Dept. Commerce, Washington, DC); General Atomic report GA-TR-3004. [2]

Fraser, A. P. (1954): 'A method of determining the electronic transition moments for diatomic molecules.' *Can. J. Phys.* **32**, 515–21 [5]

Fraser, A. R. (1966): 'The fundamental equations of radiation hydrodynamics.' UK Atomic Energy Authority report AWRE O-82/65. [2]

Freemann, B. E. (1965): 'Polarization effects on radiation diffusion in a Compton scattering medium.' General Atomic report GAMD-6157. [2]

Fried, B. D., Conte, S. D. (1961): *The Plasma Dispersion Function*. Academic Press, New York. [7]

Friedman, B., Russek, J. (1954): 'Addition theorems for sphericalwaves.' *Quart. Appl. Math.* **12**, 13–23. [5]

Frisch, M. J., Nielsen, A. B., Frisch, A. E. (1998): *Gaussian 98 Programmer's Reference.* 2^{nd} ed., Gaussian, Inc., Pittsburgh, PA. See also: www.gaussian.com. [3]

Frommhold, L., Meyer, W. (1987): 'Collision-induced rotovibrational spectra of H_2—He pairs from first principles.' *Phys. Rev. A* **35**, 632–638. [8]

Frost, B. S. (1973): 'Theory of pressure-induced absorption by symmetric top molecules.' *J. Chem. Soc. Faraday Trans. 2*, **8**, 1142–1154. [8]

Fuhr, J. R., Martin, G. A., Wiese, W. L., Younger, S. M., (1981): 'Atomic transition probabilities for iron, cobalt, and nickel. (A critical data compilation of allowed lines).' *J. Phys. Chem. Ref. Data* **10**, 305–565. [5]

Fuhr, J. R., Martin, G. A., Wiese, W. L. (1988): 'Atomic transition probabilities iron through nickel.' *J. Phys. Chem. Ref. Data* (Suppl. 4) **17**, 1–504. [5]

Fuller, K. A. (1995): 'Scattering and absorption cross sections of compounded spheres. I. Theory for external aggregation.' *J. Opt. Soc. Am. A* **11**, 3251–3260. [5]

Fuller, K. A., Kattawar, G. W. (1988a): 'Consummate solution to the problem of classical electromagnetic scattering by ensembles of spheres. I.' *Opt. Lett.* **13**, 90–92. [5]

Fuller, K. A., Kattawar, G. W. (1988b): 'Consummate solution to the problem of classical electromagnetic scattering by ensembles of spheres. II.' *Opt. Lett.* **13**, 1063–1065. [5]

Furry, W. H. (1951): 'Approximate wave functions for high energy electrons in Coulomb fields.' *Phys. Rev.* **46**, 391–396. [5]

Furssow, W., Wlassow, A. (1936): 'Zur Theorie der Verbreiterung von Spektrallinien in homogenem Gas.' *Physik Z. Sowjet Union* **10**, 378–412. [7]

Furssow, V., Wlassow, A. (1939): 'The breadth of spectral lines at large densities of a homogeneous gas.' *J. Phys. (USSR)* **1**, 335–340. [7]

Gallagher, J. W., Rumble, J. R., Beaty, E. C. (1979): 'Bibliography of Low Energy Electron and Photon Cross Section Data (January 75 through December 77).' *NBS Special Publication 426, Suppl. 1*. [6]

Gallagher, J. W., Brion, C. E., Samson, J. A. R., Langhoff, P. W. (1988): 'Absolute cross sections for molecular photoabsorption, partial photoionization, and ionic photofragmentation processes.' *J. Phys. Chem. Ref. Data* **17**, 9–153. [5]

Gamache, R. R., Lynch, R., Neshyba, S. P. (1998): 'New developments in the theory of pressure-broadening and pressure-shifting of spectral lines of H_2O: The complex Robert–Bonamy formalism.' *J. Quant. Spectr. Rad. Transfer* **59**, 319–335. [7]

Garibyan, G. M. (1953): 'Bremsstrahlung and the creation of pairs in the field of the electron.' *Zh. Eksper. Teor. Fiz.* **24**, 617–621. [5]

Gáspár, R. (1954): 'Über eine Approximation des Hartree–Fockschen Potentials durch eine universelle Potentialfunktion.' *Acta Phys. Acad. Sci. Hung.* **3**, 263–286. [3]

Gaunt, J. A. (1929): 'On the triplets of helium.' *Phil. Trans. Roy. Soc. London, Ser. A* **228**, 151–196. [5]

Gaunt, J. A. (1930): 'V. Continuous absorption.' *Phil. Trans. Roy. Soc. London, Ser. A* **229**, 163–204. [5, 6]

Gaustad, J. E. (1963): 'The opacity of diffuse cosmic matter and the early stages of star formation.' *Astrophys. J.* **138**, 1050–1073. [6]

Gear, C. W. (1971): *Numerical Initial Value Problems in Ordinary Differential Equations*. Prentice–Hall, Englewood Cliffs, NJ. [14]

Gelinas, R. J. (1971): 'Statistical aspects of the average atom model.' Lawrence Radiation Laboratory (Livermore) report UCID-15844. [4]
Gell-Mann, M., Low, F. (1951): 'Bound states in quantum field theory.' *Phys. Rev.* **84**, 350–354. [5]
Geltman, S. (1973): 'Free-free radiation in electron-neutral atomic collisions.' *J. Quant. Spectr. Rad. Transfer* **13**, 601–613. [6]
Generosa, J. J., Harris, R. A. (1970): 'Effects of high rotational quantum numbers on R–K–R F–C factors.' *J. Chem. Phys.* **53**, 3147–3152. [3]
Generosa, J. I., Harris, R. A., Sullo, L. R. (1971): 'Franck–Condon factors for various air species.' Air Force Weapons Laboratory report AFWL-TR-70-108. [5, 10]
Gérardy, G. M., Ausloos, M. (1982): 'Absorption spectrum of clusters of spheres from the general solution of Maxwell's equations. II. Optical properties of aggregated metal spheres.' *Phys. Rev. B* **25**, 4204–4229. [5]
Gerratt, J. (1971): 'General theory of spin-coupled wave functions for atoms and molecules.' *Adv. Atom. Mol. Phys.* **7**, 141–219. [3]
Gibson, G. E., Bayliss, N. S. (1933): 'Variation with temperature of the continuous absorption spectrum of diatomic molecules: Part I. Experimental, the absorption spectrum of chlorine.' *Phys. Rev.* **44**, 188–192. [6]
Gilmore, F. R. (1965): 'The contribution of generally-neglected band systems and continua to the absorption coefficient of high-temperature air.' *J. Quant. Spectr. Rad. Transfer* **5**, 125–135. [4, 7]
Gilra, D. P.(1972): 'Scientific Results from OAO.' NASA report SP-31, Washington, DC, Government Printing Office. [6]
Gingerich, O. (1970): 'The ultraviolet solar opacity.' In *International Astronomical Union Symposium No. 36, Ultraviolet Stellar Spectra and Related Ground Based Observations*. Eds. L. Houziaux, H. E. Butler; D. Reidel Publ. Co., Dordrecht-Holland, p. 140–142. [7]
Gingerich, O., Latham, D. (1970): 'The effect of silicon and carbon opacity on ultraviolet stellar spectra.' In *International Astronomical Union Symposium No. 36, Ultraviolet Stellar Spectra and Related Ground-Based Observations.* Eds. L. Houziaux, H. E. Butler; D. Reidel Publ. Co., Dordrecht-Holland, p. 64–72. [7]
Giordano, D., Capitelli, M., Colonna, G., Gorse, C. (1994): 'Tables of internal partition functions and thermodynamic properties of high-temperature air species from 50 K to 100 000 K.' European space Agency report ESA STR-237. [4]
Givens, W. (1954): 'Numerical computation of the characteristic values of a real symmetric matrix.' Oak Ridge National Laboratory report ORNL 1574. [3]
Glauber, R. J. (1963a): 'Coherent and incoherent states of the radiation field.' *Phys. Rev.* **131**, 2766–2788. [5]
Glauber, R. J. (1963b): 'Photon correlations.' *Phys. Rev. Lett.* **10**, 84–86. [5]
Godfredsen, E. (1966): 'Atomic term energies for atoms and ions with 11 to 28 electrons.' *Astrophys. J.* **145**, 308–332. [3]
Godson, W. L. (1953): 'The evaluation of infra-red radiative fluxes due to atmospheric water vapour.' *Quart. J. Roy. Met. Soc.* **79**, 367–379. [7]
Godson, W. L. (1955): 'The computation of infrared transmission by atmospheric water vapor.' *J. Meteorol.* **12**, 272–284. [7]
Goldberg, L. (1935): 'Relative multiplet strengths in LS coupling.' *Astrophys. J.* **82**, 1–25. [5]
Goldberg, L. (1936): 'Note on absolute multiplet strengths.' *Astrophys. J.* **84**, 11–13. [5]
Golden, S. A. (1962): 'Approximate spectral absorption coefficients for pure rotational transitions in diatomic molecules.' *J. Quant. Spectr. Rad. Transfer* **2**, 201–211. [7]
Golden, S. A. (1967a): 'Approximate spectral absorption coefficients of electronic transitions in diatomic molecules.' *J. Quant. Spectr. Rad. Transfer* **7**, 225–250. [7]
Golden, S. A. (1967b): 'The Doppler analog of the Elsasser band model.' *J. Quant. Spectr. Rad. Transfer* **7**, 483–494. [7]
Golden, S. A. (1968): 'The Doppler analog of the Elsasser band model – II. Integrated emissivity.' *J. Quant. Spectr. Rad. Transfer* **8**, 877–897. [7]

Golden S. A. (1969): 'The Voigt analog of an Elsasser band.' *J. Quant. Spectr. Rad. Transfer* **9**, 1067–1081. [7]

Goldman, A., Kyle, T. G. (1968): 'A comparison between statistical model and line-by-line calculations with applications to the 9.6 μm ozone and the 2.7 μm water vapor bands.' *Appl. Optics* **7**, 1167–1176. [7]

Goldstein, H. (1950): *Classical Mechanics*. Addison-Wesley Publ. Co., Inc., Reading, MA, Palo Alto, London, Dallas, Atlanta. [3]

Goldstein, R. (1964): 'Measurements of infrared absorption by water vapor at temperatures to 1000 K.' *J. Quant. Spectr. Rad. Transfer* **4**, 343–352. [11, 13]

Gombás, P. (1949): *Die Statistische Theorie des Atoms und ihre Awendungen*. Springer-Verlag, Wien. [3]

Gombás, P. (1956): 'Statistische Behandlung des Atoms.' In *Handbuch der Physik, Atome II*, XXXVI. Ed. S. Flügge; Springer-Verlag, Berlin, Göttingen, Heidelberg, p. 109–231. [3]

Goody, R. M. (1952): 'A statistical model for water vapour absorption.' *Quart. J. Roy. Met. Soc.* **78**, 165–169. [7]

Goody, R. M. (1964): *Atmospheric Radiation, I. Theoretical Basis*. Clarendon Press, Oxford. [2]

Goody, R. M., Yung, Y L. (1989): *Atmospheric Radiation: Theoretical Basis*. 2^{nd} ed., Oxford University Press, New York, Oxford. [7]

Goody, R., West, R., Chen, L., Crisp, D. (1989): 'The correlated-k method for radiation calculations in nonhomogeneous atmospheres.' *J. Quant. Spectr. Rad. Transfer* **42**, 539–550. [7]

Gordon, R. G. (1965): 'Molecular motion in infrared and Raman spectra.' *J. Chem. Phys.* **43**, 1307–1312. [5, 7]

Gordon, R. G. (1968): 'Correlation functions for molecular motion.' *Adv. Mag. Resonance* **3**, 1–42. [7]

Gordy, W., Smith, W. V., Trambarulo, R. F. (1953): *Microwave Spectroscopy*. John Wiley & Sons, Inc., New York, and Chapman & Hall, Ltd., London. [4]

Graboske Jr., H. C., Harwood, D. J., DeWitt, H. E. (1971): 'Thermodynamic properties of nonideal gases. II. The strongly ionized gas.' *Phys. Rev. A* **3**, 1419–1431. [4]

Grant, I. P. (1958): 'Calculation of Gaunt factors for free – free transitions near positive ions.' *Mon. Not. Roy. Astron. Soc.* **118**, 241–257. [7]

Grant, I. P. (1961): 'Relativistic self-consistent fields.' *Proc. Roy. Soc. (London), Ser. A* **262**, 555–576. [3]

Grant, I. P. (1992): 'Relativistic electron structure theory.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 513–518. [3, 5]

Grant, I. P. (1994): 'Relativistic electronic structure of atoms and molecules.' *Adv. Atom. Mol. Phys.* **32**, 169–186. [3]

Grant, I. P. (1996): 'Relativistic atomic structure.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 258–286. [3, 5]

Grant, W. B. (1990): 'Water vapor absorption coefficients in the 8–13 μm spectral region: A critical review.' *Appl. Optics* **29**, 451–462. [7]

Gray, C. G. (1971): 'Theory of collision-induced absorption for spherical top molecules.' *J. Phys. B* **4**, 1661–1669. [8]

Gray, L. D. (1963): 'Theoretical calculations of equilibrium infrared gas emissivities from spectroscopic data. Representative radiative energy calculations for transparent and optically dense media.' Ph. D. Thesis, California Institute of Technology. Pasadena, CA. [13]

Gray, L. D., Penner, S. S. (1965): 'Approximate band absorption calculations for methane.' *J. Quant. Spectr. Rad. Transfer* **5**, 611–620. [5, 7]

Green, J. M. (1960): 'Fermi–Dirac averages of the free-free hydrogenic Gaunt factor.' RAND Corp. report RM-2580-AEC. [6]

Green, J. M. (1964): 'The statistical mechanics of the interdependent electrons in the screening constant model of the many-electron-atom.' *J. Quant. Spectr. Rad. Transfer* **4**, 639–662. [3, 4]

Green, S. (1990): 'Raman Q-branch line shapes as a test of the H_2-Ar intermolecular potential.' *J. Chem. Phys.* **93**, 1496–1501. [7]
Green, S., Boissoles, J., Boulet, C. (1988): 'Accurate collision-induced line coupling parameters for the fundamental band of CO in He.' *J. Quant. Spectr. Rad. Transfer* **39**, 33–42. [7]
Greenberg, J. M., Libelo, L., Lind, A., Wang, R. T. (1962): 'Scattering by nonspherical particles whose size is of the order of the wave length.' *Electromagnetic Theory and Antennas Symposium*. Ed. E. C. Jordan; Pergamon Press Ltd., Oxford, England, p. 81–92. [5]
Greene, J. (1959): 'Bremsstrahlung for a Maxwellian gas.' *Astrophys. J.* **130**, 693–701. [6]
Grevesse, N. (1984): 'Accurate atomic data and solar photospheric spectroscopy.' *Phys. Scripta* **T8**, 49–58. [13]
Grevesse, N., Sauval, A. J., van Dishoeck, E. F. (1984): 'An analysis of vibration–rotation lines of OH in the solar infrared spectrum.' *Astron. Astrophys.* **141**, 10–16. [5, 13]
Griem, H. R. (1962): 'Wing formulae for Stark broadened hydrogen and hydrogenic lines.' *Astrophys. J.* **136**, 422–430. [7]
Griem, H. (1964): *Plasma Spectroscopy*. McGraw-Hill Book Co., Inc., New York, San Francisco, Toronto, London. [4, 5, 7, 12, 13]
Griem, H. R. (1974): *Spectral line broadening by plasmas.* Academic Press, New York, London. [7]
Griem, H. R., Shen, K. Y. (1961): 'Stark broadening of hydrogenic ion lines in a plasma.' *Phys. Rev.* **122**, 1490–1496. [7]
Griem, H. R., Baranger, M., Kolb, A. C., Oertel, G. (1962): 'Stark broadening of neutral helium lines in a plasma.' *Phys. Rev.* **125**, 177–195. [7]
Grimaldi, F., Grimaldi-Lecourt, A. (1982): 'Quasi-static electron density fluctuations of atoms in hot compressed matter.' *J. Quant. Spectr. Rad. Transfer* **27**, 373–385. [3, 4]
Gross, E. P. (1955): 'Shape of collision-broadened spectral lines.' *Phys. Rev.* **97**, 395–403. [7]
Gross, E. K. U. (2009): Websites: http://users.physik.fu-berlin.de/~ag-gross/ and http://online.itp.ucsb.edu/online/cem02/gross/. [3]
Gross, E. K. U., Dreizler, R. M. (Eds.) (1995): *Density Functional Theory.* Proc. NATO Advanced Study Institute. Plenum ASI series B **337**, Spinger-Verlag New York. [3]
Gross, E. K. U., Toepfer, A., Jacob, B., Horbatsch, M., Luedde, H. J., Dreizler, R. M. (1983): 'Density functional approach to molecular structure and atomic scattering.' In *Molecular Ions, Geometric and Electronic Structures,* Eds. J. Berkowitz and K. O. Groeneveld, Plenum Press, New York, p. 419–422. [3]
Gruner, D., Brumer, P. (1987): 'Efficient evaluation of harmonic polyatomic Franck–Condon factors.' *Chem. Phys. Lett.* **138**, 310–314. [5]
Guest, M. F., Wilson, S. (1981): 'The use of vector processors in quantum chemistry: Experience in the U. K.' In *Supercomputers in Chemistry*. Eds. P. Lykos and I. Shavitt; ACS Symposium Ser. **173**, Am. Chem. Soc. Washington. [3]
Gustafson, B. Å. S. (1996): 'Microwave analog to light scattering measurements: A modern implementation of a proven method to achieve precise control.' *J. Quant. Spectr. Rad. Transfer* **55**, 663–672. [5]
Gustafsson, B., Bell, R. A., Eriksson, K., Nordlund, Å. (1975): 'A grid of madel atmospheres for metal-deficient giant stars I.' *Astron. Astrophys.* **42**, 407–432. [7]
Gustafsson, T., Levinson, H. J. (1981): 'Shape resonances in diatomic molecules: NO.' *Chem. Phys. Lett.* **78**, 28–31. [5]
Gyldén, N., Einarsson, B. (1969): 'Classical calculation of inverse bremsstrahlung cross sections in screened potentials.' *J. Quant. Spectr. Rad. Transfer* **9**, 1117–1132. [6]
Hakel, P., Sherrill, M. E., Mazevet, S., Abdallah Jr., J., Colgan, J., Kilcrease, D. P., Magee, N. H., Fontes, C. J., Zhang, H. L. (2006): 'The new Los Alamos opacity code ATOMIC.' *J. Quant. Spectr. Rad. Transfer* **99** 265–271. [14]
Hakim, R., Mangeney, A. (1971): 'Collective oscillations of a relativistic radiating electron plasma.' *Phys. Fluids* **14**, 2751–2761. [6]
Hamermesh, M. (1962): *Group Theory and Its Application to Physical Problems*. Addison-Wesley Publ. Co., Reading, MA, London. [7]

Hamilton, D. R. (1947): 'The resonance radiation induced by elliptically polarized light.' *Astrophys. J.* **106**, 457–465. [5]

Hammond, B. L., Lester, Jr., W. A., Reynolds, P. J. (1994): *Monte Carlo Methods in Ab-Initio Quantum Chemistry.* World Scientific, London, Singapore, River Edge, New Jersey. [3]

Hansen, J. P. (1973): 'Statistical mechanics of dense ionized matter. I. Equilibrium properties of the classical one-component plasma.' *Phys. Rev. A* **8**, 3096–3109. [6]

Hansen, W. W. (1935): 'A new type of expansion in radiation problems.' *Phys. Rev.* **47**, 139–143. [5]

Harris III, D. L. (1948): 'On the line-absorption coefficient due to Doppler effect and damping.' *Astrophys. J.* **108**, 112–115. [7]

Harris, F. E. (1960): 'Molecular orbital studies of diatomic molecules. I. Method of computations of heteronuclear systems.' *J. Chem. Phys.* **32**, 3–18. [3]

Harris, F. E. (1967): 'Open-shell orthogonal molecular orbital theory.' *J. Chem. Phys.* **46**, 2769–2776. [3]

Harris, R., Blackledge, M., Generosa, J. (1969): 'Rydberg–Klein–Rees F–C factors for the O_2 Schumann-Runge system including high vibrational quantum numbers.' *J. Mol. Spectr.* **30**, 506–512. [3]

Harrison, A. J., Cederholm, B. J., Terwilliger, M. A. (1959): 'Absorption of acyclic oxygen compounds in the vacuum ultraviolet. I. Alcohols.' *J. Chem. Phys.* **30**, 355–356. [5]

Harter, W. G. (1996): 'Molecular symmetry and dynamics.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 378–393. [3]

Harter, W. G., Patterson, C. W., da Paixao, F. J. (1978): 'Frame transformation relations and multipole transitions in symmetric polyatomic molecules.' *Rev. Mod. Phys.* **50**, 37–83. [3]

Hartmann, J. M., Taine, J., Bonamy, J., Labani, B., Robert, D. (1987): 'Collisional broadening of rotation–vibration lines for asymmetric–top molecules. II. H_2O diode laser measurements in the 400–900 K range; calculations in the 300–2000 K range.' *J. Chem. Phys.* **86**, 144–156. [7]

Hartree, D. R. (1957): *The Calculation of Atomic Structures*. John Wiley & Sons, Inc., New York; Chapman & Hall, Ltd., London. [3]

Hartree, D. R. (1958): *Numerical Analysis*. 2^{nd} ed., Oxford University Press, London. [4]

Hauschildt, P. H. (1992): 'A fast operator perturbation method for the solution of the special relativistivc equation of radiative transfer in spherical symmetry.' *J. Quant. Spectr. Rad. Transfer* **47**, 433–453. [14]

Hauschildt, P. H. (1993): 'Multi-level non-LTE radiative transfer in expanding shells.' *J. Quant. Spectr. Rad. Transfer* **50**, 301–318. [14]

Hauschildt, P. H., Störzer, H., Baron, E. (1994): 'Convergence properties of the accelerated Λ-iteration method for the solution of radiative transfer problems.' *J. Quant. Spectr. Rad. Transfer* **51**, 875–891. [14]

Hauschildt, P. H., Starrfield, S., Shore, S. N., Allard, F., Baron, E. (1995): 'The physics of early nova spectra.' *Astrophys. J.* **447**, 829–847. [14]

Hauschildt, P. H., Baron, E., Starrfield, S., Allard, F. (1996): 'The effect of Fe II non-LTE on nova atmospheres and spectra.' *Astrophys. J.* **462**, 386–403. [14]

Hauschildt, P. H., Allard, F., Alexander, D. R., Baron, E. (1997a): 'Non-local thermodynamic equilibrium effects of Ti I in M dwarfs and giants.' *Astrophys. J.* **488**, 428–442. [14]

Hauschildt, P. H., Baron, E., Allard, F. (1997b): 'Parallel implementation of the PHOENIX generalized stellar atmosphere program.' *Astrophys. J.* **483**, 390–398. [14]

Hauschildt, P. H., Lowenthal, D. K., Baron, E. (2001): 'Parallel implementation of the PHOENIX generalized stellar atmosphere program. III. A parallel algorithm for direct opacity sampling.' *Astrophys. J. Suppl. Ser.* **134**, 323–329. [14]

Hay, P. J. (1981): 'Electronic structure of molecules using relativistic effective core potentials.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 383–402. [3]

Head-Gordon, M., Artacho, E. (2008): 'Chemistry on the computer.' *Phys. Today* April, 58–63. [3]

Heaps, H. S., Herzberg, G. (1952): 'Intensity distribution in the rotation–vibration spectrum of the OH molecule.' *Z. Physik* **133**, 48–64. [5]

Hefferlin, R., Kuznetsova, L. A. (1999): 'Systematics of diatomic molecular transition moments.' *J. Quant. Spectr. Rad. Transfer* **62**, 765–774. [3, 5]
Hehre, W. J. (1986): *Ab Initio Molecular Orbital Theory.* Wiley, New York. [3]
Heitler, W. (1954). *The Quantum Theory of Radiation*. Clarendon Press, Oxford. [5, 7]
Helgaker, T. (1992): 'Calculation of geometrical derivatives in molecular electronic structure theory.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 353–422. [5]
Heller, E. J. (1981): 'The semiclassical way to molecular spectroscopy.' *Acc. Chem. Res.* **14**, 368–375. [5]
Henke, B. L., Elgin, R. L. (1970): 'X-ray absorption tables for the 2-to-200 Å region.' In *Advances in X-Ray Analysis* **13**. Eds. B. L. Henke, J. B. Newkirk, G. R. Mallett; Plenum Press, New York, NY, p. 639–665. [5]
Herman, F., Skillman, S. (1963): *Atomic Structure Calculations*. Prentice Hall, Inc., Englewood Cliffs, NJ. [3]
Herman, R. C., Wallis, R. F. (1955): 'Influence of vibration–rotation interaction on line intensities in vibration–rotation bands of diatomic molecules.' *J. Chem. Phys.* **23**, 637–646. [5, 7]
Hermann, M. R. (1984): 'Explicit Hilbert-space representations of atomic and molecular photoabsorption spectra.' Ph. D. Dissertation, Indiana University, Bloomington, IN. [5]
Herzberg, G. (1945): *Molecular Spectra and Molecular Structure. II. Infrared and Raman Spectra of Polyatomic Molecules*. D. Van Nostrand Co., Inc., Princeton, NJ, Toronto, London, New York. [3, 4, 5]
Herzberg, G. (1950): *Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules*. D. van Nostrand Co., Inc., Princeton, NJ, Toronto, London, New York. [3, 4, 5]
Herzberg, G. (1966): *Molecular Spectra and Molecular Structure. III. Electronic Spectra and Electronic Structure of Polyatomic Molecules*. D. van Nostrand Co., Inc., Princeton, NJ, Toronto, London, New York. [3, 5, 7]
Hess Jr., B. A., Schaad, L. J., Čársky, P., Zahradník, R. (1986): 'Ab initio calculations of vibrational spectra and their use in the identification of unusual molecules.' *Chem. Rev.* **86**, 709–730. [5]
Hesser, J. E. (1968): 'Absolute transition probabilities in ultraviolet molecular spectra.' *J. Chem. Phys* **48**, 2518–2535. [5]
Hibbert, A. (1975): 'CIV3 – A general program to calculate configuration interaction wave functions and electric-dipole oscillator strengths.' *Comp. Phys. Comm.* **9**, 141–172. [3]
Hinderling, J., Sigrist, M. W., Kneubühl, F. K. (1987): 'Laser-photoacoustic spectroscopy of water-vapor continuum and line absorption in the 8–14 μm atmospheric window.' *Infrared Phys.* **27**, 63–120. [7]
Hilborn, R. C. (1982): 'Einstein coefficients, cross sections, f values, dipole moments, and all that' *Am. J. Phys.* **50**, 982–986; updated: http://arxiv.org/abs/physics/0202029. [5]
Hirota, F. (1976): 'Calculation of the molecular photoionization cross sections in the UV region. I. Diatomic molecules.' *J. Electron Spectr. Related Phenom.* **9**, 149–167. [5]
Hirschfelder, J. O., Magee, J. L. (1945): 'Opacity and thermodynamic properties of air at high temperatures.' Los Alamos Scientific Laboratory report LA-296. [1]
Hirschfelder, J. O., Curtiss, C. F., Bird, R. B. (1954): *Molecular Theory of Gases and Liquids*. J. Wiley & Sons, Inc., New York, Chapman & Hall, Limited, London. [9]
Hjerting, F. (1938): 'Tables facilitating the calculation of line absorption coefficients.' *Astrophys. J.* **88**, 508–515. [7]
Hochstrasser, UẆ. (1972): 'Orthogonal Polynomials,' Chap. 22 In *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Abramowitz, M., Stegun, I. A., (Eds.) (1972), NBS Applied Mathematics Series **55**, U.S. Dept. Commerce, Washington, DC. Tenth printing, December 1972, with corrections. [13]
Hönl, H. (1926): 'Zum Intensitätsproblem der Spektrallinien.' *Ann. Phys. Ser. 4* **79**, 273–323. [5]
Hönl, H., London, F. (1925): 'Über die Intensitäten der Bandenlinien.' *Z. Phys.* **33**, 803–809. [5]
Hohenberg, P., Kohn, W. (1964): 'Inhomogeneous Electron Gas.' *Phys. Rev. B* **136**, 864–871. [3]

Hollstein, M., Lorents, D. C., Peterson, J. R., Sheridan, J. R. (1969): 'Time of flight measurement of N_2 and N_2^+ lifetimes.' *Can. J. Chem.* **47**, 1858–1861. [5]
Holtsmark, J. (1919a): 'Über die Verbreiterung von Spektrallinien.' *Ann. Physik* **58**, 577–630. [7]
Holtsmark, J. (1919b): 'Über die Verbreiterung von Spektrallinien.' *Physik. Z.* **20**, 162–168. [7]
Holtsmark, J. (1924): 'Über die Verbreiterung von Spektrallinien. II.' *Physik. Z.* **25**, 73–84. [7]
Holweger, H., Müller, E. A. (1974): 'The photospheric barium spectrum: Solar abundance and collision broadening of Ba II lines by hydrogen.' *Solar Physics* **39**, 19–30. [5]
Hottel, H. C. (1954): 'Radiant heat transfer.' In *Heat Transmission.* Ed. W. H. McAdams; 3^{rd} ed., McGraw-Hill Book Co., Inc., New York, p. 55–125. [7]
Houdeau, J. P., Boulet, C., Robert, D. (1985): 'A theoretical and experimental study of the infrared line shape from resonance to the wings for uncoupled lines.' *J. Chem. Phys.* **82**, 1661–1673. [7]
Hougen, J. T., Watson, J. K. G. (1965): 'Anomalous rotational line intensities in electronic transitions of polyatomic molecules: Axis-switching.' *Can. J. Phys.* **43**, 298–320. [5, 7]
Hougen, J. T., Bunker, P. R., Johns, J. W. C. (1970): 'The vibration–rotation problem in triatomic molecules allowing for a large-amplitude bending motion.' *J. Mol. Spectr.* **34**, 136–172. [3]
Hoy, A. R., Bunker, P. R. (1974): 'The effective rotation-bending Hamiltonian of a triatomic molecule and its application to extreme centrifugal distortion in the water molecule.' *J. Mol. Spectr.* **52**, 439–456. [3]
Hoy, A. R., Mills, I. M., Strey, G. (1972): 'Anharmonic force constant calculations.' *Mol. Phys.* **24**, 1265–1290. [3]
Hsu, D. K. (1981): 'Experimental lifetimes, F–C factors, and vibrational and rotational oscillator strengths.' In *Handbook of Spectroscopy.* III. Ed. J. W. Robinson, CRC Press, Boca Raton, p. 269–402. [5]
Hubač, I., Svrček, M. (1992): 'Many-body perturbation theory for vibrational-electronic molecular Hamiltonian.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 471–512. [3]
Hubbard, W. B. (1966): 'Studies in stellar evolution. V. Transport coefficients of degenerate stellar matter.' *Astrophys. J.* **146**, 858–870. [9]
Hubbard, W. B., Lampe, M. (1969): 'Thermal conduction by electrons in stellar matter.' *Astrophys. J. Suppl. Ser.* **18**, 297–346. [9]
Huber, D. L., van Vleck, J. H. (1966): 'The role of Boltzmann factors in line shape.' *Rev. Mod. Phys.* **38**, 187–204. [8]
Huber, K. P., Herzberg, G. (1979): *Molecular Spectra and Molecular Structure: IV. Constants of Diatomic Molecules*. Van Nostrand Reinhold Co., New York. [3]
Huebner, W. F. (1967): 'Some estimates of the radiative Rosseland mean opacity.' *J. Quant. Spectr. Rad. Transfer* **7**, 943–949. [11]
Huebner, W. F. (1968): 'Electron–Electron Interaction from Single-Electron Theory.' Los Alamos Scientific Laboratory report LA-3899. [3]
Huebner, W. F. (1970): 'Electron–electron interaction in energy level determination.' *J. Quant. Spectr. Rad. Transfer* **10**, 949–973; **11**, 142. [3]
Huebner, W. F. (1986): 'Atomic and Radiative Processes in the Solar Interior.' In *Physics of the Sun*. Ed. P. A. Sturrock; D. Reidel Publishing Co., Dordrecht, Boston, Lancaster, Tokyo, Vol. 1, p. 33–75. [1, 6, 13]
Huebner, W. F., Fullerton, L. W. (1974): 'Status of molecular opacities of interest in the modeling of a proto-solar nebula.' In *Exploration of the Planetary System*, Eds. A. Woszczyk and C. Iwaniszewska. IAU Symposium 65, Torun, Poland, D. Reidel Pub. Co. Dordrecht-Holland, Boston, p. 13–20. [2]
Huebner, W. F., Stuart, R. S. (1964): 'Status Report on Opacity Calculations.' Los Alamos Scientific Laboratory report LAMS-3002. [5]
Huebner, W. F., Stuart, R. S. (1965): 'Status Report on Opacity Calculations.' Los Alamos Scientific Laboratory report LAMS-3002 Suppl. I. [5]
Huebner, W. F., Mayer, H., Meyerott, R. E., Penner, S. S., (Eds.) (1965): 'Opacities. Proceedings of the second international conference.' *J. Quant. Spectr. Rad. Transfer* **5**, 1–280. [1, 13]

Huebner, W. F., Generosa, J., Harris, R. (1967): 'Status Report on Opacity Calculations.' Los Alamos Scientific Laboratory report LA-3002-MS Suppl. II. [5]
Huebner, W. F., Merts, A. L., Magee Jr., N. H., Argo, M. F. (1977): Astrophysical Opacity Library. Los Alamos Scientific Laboratory report LA-6760-M. [10]
Huebner, W. F., Keady, J. J., Lyon, S. P. (1992): 'Solar Photo Rates for Planetary Atmospheres and Atmospheric Pollutants.' *Astrophys. Space Sci.* **195**, 1–294. [4, 5]
Huffman, R. E., Tanaka, Y., Larrabee, J. C. (1963): 'Absorption coefficients of xenon and argon in the 600–1025 Å wavelength regions.' *J. Chem. Phys.* **39**, 902–909. [5]
Hummer, D. G. (1962): 'Non-coherent scattering.' *Mon. Not. Roy. Astron. Soc.* **125**, 21–37. [7]
Hummer, D. G. (1965): 'The Voigt function. An eight-significant-figure table and generating procedure.' *Memoirs, Roy. Astron. Soc.* **70**, 1–31. [7]
Hummer, D. G. (1991): 'The opacity project and the practical utilization of atomic data.' In *Stellar Atmospheres: Beyond Classical Models*, Eds. L. Crivellari, I. Hubeny, and D. G. Hummer; Kluwer Academic Publ., p. 431–439. [1, 3]
Hummer, D. G., Mihalas, D. (1988): 'The equation of state for stellar envelopes. I. An occupation probability formalism for the truncation of internal partition functions.' *Astrophys. J.* **331**, 794–814. [4]
Hund, F. (1925a): 'Zur Deutung verwickelter Spektren, insbesondere der Elemente Scandium bis Nickel.' *Z. Physik* **33**, 345–371. [7]
Hund, F. (1925b): 'Zur Deutung verwickelter Spektren. II.' *Z. Physik* **34**, 296–308. [7]
Hundley, R. O. (1962): 'Bremsstrahlung During the Collision of Low-Energy Electrons with Neutral Atoms and Molecules.' Rand Corporation report RM 3334-ARPA. [6]
Hüpper, B., Eckhardt, B. (1999): 'Uniform semiclassical calculation of the direct part of the photodissociation cross section of water.' *J. Chem. Phys.* **110**, 11749–11755. [5]
Hüpper, B., Eckhardt, B., Engel, V. (1997): 'Semiclassical photodissociation cross section for H_2O.' *J. Phys. B* **30**, 3191–3209. [5]
Hurley, A. C. (1962): 'Equivalence of Rydberg–Klein–Rees and simplified Dunham potentials.' *J. Chem. Phys.* **36**, 1117–1118. [3]
Hurley, A. C. (1976a): *Introduction to the Electron Theory of Small Molecules.* Academic Press, London, New York, p. 165–168. [3]
Hurley, A. C. (1976b): *Electron Correlation in Small Molecules.* Theoretical Chemistry Monographs **6**. Academic Press, London, New York. [3, 5]
Iachello, F., Levine, R. D. (1995): *Algebraic Theory of Molecules*. Oxford University Press. [5]
Iben Jr., I. (1968): 'Electron conduction in Red Giants.' *Astrophys. J.* **154**, 557–579. [9]
Iben Jr., I. (1975): 'Thermal pulses; p-capture, α-capture s-process nucleosynthesis; and convective mixing in a star of intermediate mass.' *Astrophys. J.* **196**, 525–547. [9]
Iglesias, C. A., Rogers, F. J. (1991): 'Opacities for the solar radiative interior.' *Astrophys. J.* **371**, 408–417. [13]
Iglesias, C. A., Rogers, F. J. (1996): 'Updated Opal Opacities.' *Astrophys. J.* **464**, 943–953. [13]
Infeld, L. (1947): 'The influence of the width of the gap upon the theory of antennas.' *Quart. Appl. Math.* **5**, 113–132. [5]
Inglis, D. R. (1931): 'Energy relations in complex spectra.' *Phys. Rev.* **38**, 862–872. [3]
Ishikawa, Y., Malli, G. L. (1981): 'Fully relativistic effective core potentials (FRECP).' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 363–382. [3]
Ishikawa, Y., Kaldor, U. (1996): 'Relativistic many-body calculations on atoms and molecules.' In *Computational Chemistry: Reviews of Current Trends.* Ed., J. Leszczynski, World Scientific, Singapore, New Jersey, London, Hong Kong, Bangalore, Taipei., p. 1–52. [3]
Islampour, R. (1989): 'Electronic spectral line shape of a polyatomic molecule.' *Chem. Phys.* **133**, 425–435. [7]
Islampour, R., Kasha, M. (1983a): 'Molecular translational-rovibronic Hamiltonian. I. Non-linear molecules.' *Chem. Phys.* **74**, 67–76. [7]
Islampour, R., Kasha, M. (1983b): 'Molecular translational-rovibronic Hamiltonian. II. Linear molecules.' *Chem. Phys.* **75**, 157–164. [7]

Islampour, R., Lin, S. H., (1991): 'A new expression for multidimensional F–C integrals.' *Trends Chem. Phys.* **1** 249–275. [5]

Islampour, R., Sutcliffe, B. T. (1987): 'Theories of electronic spectral bandshape functions of molecules.' *Iran J. Chem. - Chem. Eng.* **9**, 3–25. [7]

Islampour, R., Dehestani, M., Lin, S. H. (1999): 'A new expression for multidimensional Franck–Condon integrals.' *J. Mol. Spectr.* **194**, 179–184. [5]

Isnard, P., Boulet, C., Robert, D., Galatry, L. (1977): 'Line-widths in the vibration–rotation spectra of diatomic molecules perturbed by tetrahedral molecules.' *Mol. Phys.* **33**, 259–280. [7]

Isobe, S. (1971): 'Graph of scattering for spherical particles and application to interstellar extinction.' *Ann. Tokyo Astron. Obs.* **12**, 263–285. [5]

Itikawa, Y. (1978a): 'Vibrational-rotational structure in the angular distribution and intensity of photoelectrons from diatomic molecules.' *Chem. Phys.* **28**, 461–471. [5]

Itikawa, Y. (1978b): 'Vibrational-rotational structure in the angular distribution and intensity of photoelectrons from diatomic molecules. II. H_2.' *Chem. Phys.* **30**, 109–117. [5]

Itikawa, Y. (1987): 'Asymmetry parameters of the angular distribution of photoelectrons form the hydrogen molecule.' *Comments At. Mol. Phys.* **20**, 51–62. [5]

Itikawa, Y., Hayashi, M., Ichimura, A., Onda, K., Sakimoto, K. Takayanagi, K., Nakamura, M., Nishimura, H., Takayanagi, T. (1986): 'Cross sections for collisions of electrons and photons with nitrogen molecules.' *J. Phys. Chem. Ref. Data* **15**, 985–1010. [6]

Itoh, N., Kohyama, Y. (1993): 'Electrical and thermal conductivities of dense matter in the crystalline lattice phase. II. Impurity scattering.' *Astrophys. J.* **404**, 268–270. [9]

Itoh, N., Kohyama, Y. (1994): 'Electrical and thermal conductivities of dense matter in the crystalline lattice phase. II. Impurity scattering.' *Astrophys. J.* **420**, 943. [9]

Itoh, N., Mitake, S., Iyetomi, H., Ichimaru, S. (1983): 'Electrical and thermal conductivities of dense matter in the liquid metal phase. I. High-temperature results.' *Atrophys. J.* **273**, 774–782. [9]

Itoh, N., Kohyama, Y., Matsumoto, N., Seki, M. (1984): 'Electrical and thermal conductivities of dense matter in the crystalline lattice phase.' *Astrophys. J.* **285**, 758–765. [9]

Itoh, N., Nakagawa, M., Kohyama, Y. (1985): 'Relativistic free–free opacity for high-temperature stellar plasma.' *Astrophys. J.* **294**, 17–22. [6]

Itoh, N., Kojo, K., Nakagawa, M. (1990): 'Relativistic free–free Gaunt factor of the dense high-temperature stellar plasma. II. Carbon and oxygen plasmas.' *Astrophys. J. Suppl. Ser.* **74**, 291–314. [6]

Itoh, N., Hayashi, H., Kohyama, Y. (1993): 'Electrical and thermal conductivities of dense matter in the crystalline lattice phase. III. Inclusion of lower densities.' *Astrophys. J.* **418**, 405–413. [9]

Itoh, N., Hayashi, H., Kohyama, Y. (1994): 'Electrical and thermal conductivities of dense matter in the crystalline lattice phase. III. Inclusion of lower densities.' *Astrophys. J.* **436**, 418. [9]

Itoh, N., Sakamoto, T., Kusano, S., Nozawa, S., Kohyama, Y. (2000): 'Relativistic thermal bremsstrahlung Gaunt factor for the intracluster plasma. II. Analytic fitting formulae.' *Astrophys. J. Suppl. Ser.* **128**, 125–138. [6]

Iwata, S., Nagukura, S. (1974): 'Theoretical study of the photoelectron intensities and angular distributions.' *Mol. Phys.* **27**, 425–440. [5]

Jackson, J. D. (1962): *Classical Electrodynamics.* John Wiley & Sons, New York, p. 459. [9]

Jacobsohn, B. A. (1947): 'The opacity of uranium at high temperature.' Ph. D. Dissertation, Dept. Physics, University of Chicago, Chicago, IL. [1, 5, 7]

Jahn, H. A., Hope, J. (1954): 'Symmetry properties of the Wigner 9j symbol.' *Phys. Rev.* **93**, 318–321. [5]

Jahoda, F. C., Sawyer, G. A. (1971): 'Optical refractivity of plasmas.' *Methods of Experimental Physics*, Vol. 9B. Ed. L. Marton; Academic Press, New York, London. [13]

Jarmain, W. R. (1959): 'Simplified analytical representation of Klein-Dunham potential energy functions.' *J. Chem. Phys.* **31**, 1137–1138. [3]

Jarmain, W. R. (1960): 'Klein-Dunham potential energy functions in simplified analytical form.' *Can. J. Phys.* **38**, 217–230. [3]

Jarmain, W. R., Nicholls, R. W. (1964): 'A theoretical study of the O_2 $X^3\Sigma_g^- - B^3\Sigma_u^-$ photodissociation continuum.' *Proc. Phys. Soc. (London)* **84**, 417–424. [5]

Jarmain, W. R., Fraser, P. A., Nicholls, R. W. (1953): 'Vibrational transition probabilities of diatomic molecules: Collected results N_2, N_2^+, NO, O_2^+.' *Astrophys. J.* **118**, 228–233. [11]

Jauch, J. M., Rohrlich, F. (1976): *The Theory of Photons and Electrons*. 2^{nd} ed., Springer-Verlag, New York, Heidelberg. [5]

Jefferies, J. T. (1968): *Spectral Line Formation*. Blaisdell Publ. Co., Waltham, MA, Toronto, London. [7]

Jensen, H. (1934): 'Interchange in the Thomas–Fermi atom.' *Z. Physik* **89**, 713–719. [3]

Jensen, P. (1983): 'The non-rigid bender Hamiltonian for calculating the rotation–vibration energy levels of a triatomic molecule.' *Comp. Phys. Rep.* **1**, 1–55. [3]

Jensen, P. (1992): 'Calculation of molecular rotation–vibration energies directly from the potential energy function.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 423–470. [3]

Jeunehomme, M. (1966): 'Transition moment of the first positive band system of nitrogen.' *J. Chem. Phys.* **45**, 1805–1811. [5]

Joens, J. A. (1987): 'Gaussian approximation for the temperature dependence of a continuous electronic spectrum.' *Chem. Phys. Lett.* **138**, 512–515. [6]

Jørgensen, U. G., Almlöf, J., Gustafsson, B., Larsson, M., Siegbahn, P. (1985): 'CASSCF and CCI calculations of the vibrational band strengths of HCN.' *J. Chem. Phys.* **83**, 3034–3041. [5]

Jørgensen, U. G., Almlöf, J., Siegbahn, P. E. M. (1989): 'Complete active space self-consistent field calculations of the vibrational band strength for C_3.' *Astrophys. J.* **343**, 554–561. [5]

John, I. G., Bacskay, G. Z., Hush, N. S. (1980): 'Finite field method calculations. VI. Raman scattering activities, infrared absorption intensities and higher-order moments: SCF and CI calculations for the isotopic derivatives of H_2O and SCF calculation for CH_4.' *Chem. Phys.* **51**, 49–60. [5]

Johnson, C. R. (1949): *An Introduction to Molecular Spectra*. Pitman Publ. Corp., New York, London. [5]

Johnson, H. R., Krupp, B. M. (1976): 'Treatment of atomic and molecular line blanketing by opacity sampling.' *Astrophys. J.* **206**, 201–207. [7]

Johnson, H. R., Collins, J. G., Krupp, B., Bell, R. A. (1977): 'The line blanketing and structure of the atmosphere of Arcturus.' *Astrophys. J.* **212**, 760–767. [7]

Johnson, K. H. (1973): 'Scattered-wave theory of the chemical bond.' *Adv. Quantum Chem.* **7**, 143–185. [3]

Johnson, W. R. (1998): 'Relativistic many-body perturbation theory for highly charged ions.' In *Many-Body Atomic Physics*. Eds. J. J. Boyle and M. S. Pindzola; Cambridge University Press, Cambridge, New York, Melbourne, p. 39–64. [3]

Johnston, R. R., Landshoff, R. K. M., Platas, O. R. (1972): 'Radiative properties of high temperature air,' Lockheed Palo Alto Research Laboratory report LMSC D267205. [3, 7]

Jones, T. W., Merrill, K. M. (1976): 'Model dust envelopes around late-type stars.' *Astrphys. J.* **209**, 509–524. [6]

Jones, W. W. (1973): 'Comparison of measured and calculated Stark parameters for singly ionized atoms.' *Phys. Rev. A* **7**, 1826–1832. [12]

Julienne, (1985): 'Collision-induced radiative transitions at optical frequencies.' In *Phenomena Induced by Intermolecular Interactions*. Ed. G. Birnbaum; Plenum Press, New York, London, p. 749–772. [8]

Jungen, C., Ross, S. C. (1997): 'Unified quantum-defect theory treatment of molecular ionization and dissociation.' *Phys. Rev. A* **55**, 2503–2506. [5]

Kähler, H. (1971): 'The computation of photoionization cross sections by means of the scaled Thomas–Fermi potential.' *J. Quant. Spectr. Rad. Transfer* **11**, 1521–1535. [12]

Kähler, H. (1973): 'A simplified Hartree–Fock method for opacity calculations.' *J. Quant. Spectr. Rad. Transfer* **13**, 401–416. [3]

Kahn, F. D. (1959): 'Long-range interactions in ionized gases in thermal equilibrium.' *Astrophys. J.* **129**, 205–216. [6]

Kalkofen, W., (Ed.) (1984): *Methods of Radiative Transfer*. Cambridge University Press, Cambridge, New York, New Rochelle, Melbourne, Sydney. [2]

Kalkofen, W., (Ed.) (1987): *Numerical Radiative Transfer*. Cambridge University Press, Cambridge, New York, New Rochelle, Melbourne, Sydney. [2]

Kaplan, G. (1975): *Symmetry of Many-Electron Systems*. Academic Press, London, New York. [3]

Kaplan, L. D. (1953): 'Regions of validity of various absorption coefficient approximations.' *J. Atmos. Sci.* **10**, 100–104. [7]

Karwowski, J. (1992): 'The configuration interaction approach to electron correlation.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 65–98. [3]

Karwowski, J., Planelles, J., Rajadell, F. (1997): 'Average energy of an N-electron system in a finite-dimensional and spin-adapted model space.' *Int. J. Quantum Chem.* **61**, 63–65. [3]

Karzas, W. J., Latter, R. (1961): 'Electron radiative transitions in a Coulomb field.' *Astrophys. J. Suppl. Ser.* **6**, 167–212. [5, 6]

Kassel, L. S. (1936): 'The calculation of thermodynamic functions from spectroscopic data.' *Chem. Rev.* **18**, 277–313. [4]

Kato, S., Ackerman, T. P., Mather, J. H., Clothiaux, E. E. (1999): 'The k-distribution method and correlated-k approximation for a shortwave radiative transfer model.' *J. Quant. Spectr. Rad. Transfer* **62**, 109–121. [7]

Kattawar, G. W., Humphreys, T. J. (1980): 'Electromagnetic scattering from two identical pseudospheres.' In *Light Scattering by Irregular Shaped Particles*, Ed. D. W. Schuerman, Plenum Press, New York, London, p. 177–190. [5]

Keady, J. J., Huebner, W. F., Abdallah Jr., J., Magee Jr., N. H. (1990): 'Progress in LTE and non-LTE radiative transport properties.' In *Physical Processes in Hot Cosmic Plasmas*. Eds. W. Brinkmann, A. C. Fabian, F. Giovannelli; NATO ASI Ser. C. **305**, p. 181–195. [6]

Keck, J. C., Camm, J. C., Kivel, B., Wentink Jr., T. (1959): 'Radiation from hot air. Part II. Shock tube study of absolute intensities.' *Ann. Phys. N. Y.* **7**, 1–38. [7]

Keck, J. C., Allen, R. A., Taylor, R. L. (1963): 'Electronic transition moments for air molecules.' *J. Quant. Spectr. Rad. Transfer* **3**, 335–353. [5]

Keller, G., Meyerott, R. E. (1952): 'The ionization of gas mixtures in stellar interiors.' Argonne National Laboratory report ANL-4771. [4]

Kelly, H. P. (1963): 'Correlation effects in atoms.' *Phys. Rev.* **131**, 684–699. [5]

Kelly, H. P. (1968): 'Correlation structure in atoms.' *Advances in Theoretical Physics.* Ed. K. A. Brueckner; Academic Press, New York, London, Vol. 2, p. 75–169. [5]

Kelly, H. P. (1969): 'Applications of many-body diagram techniques in atomic physics.' In *Advances in Chemical Physics. (Correlation Effects in Atoms and Molecules).* Eds. R. Lefebvre, C. Moser; Interscience Publishers - John Wiley & Sons, Ltd., London, New York, Sydney, Toronto, Vol. 14, p. 129–190. [5]

Kemper, M. J. H., van Dijk, J. M. F., Buck, H. M. (1978): 'A backtracking algorithm for exact counting of internal molecular energy levels.' *Chem. Phys. Lett.* **53**, 121–124. [7]

Kendall, M. G., Stuart, A. (1963): *Advanced Theory of Statistics.* Vol. 1. *Distribution Theory.* 2^{nd} ed., Charles Griffin and Company Limited, London. [7]

Kerker, M. (1969): *The Scattering of Light and Other Electromagnetic Radiation*. Academic Press, New York. [5]

Kieffer, L. J. (1976): 'Bibliography of Low Energy Electron and Photon Cross Section Data (through December 1974): Final Report.' *U. S. N. B. S. Special Publication 426.* [6]

Kilcrease, D. P. (2007): Private communication. [6]

Kilcrease, D. P., Magee Jr., N. H. (2001): 'Plasma non-ideality effects on the photo-electron scattering contribution to radiative opacity.' *J. Quant. Spectr. Rad. Transfer* **71**, 445–453. [6]

Kim, D-S. (2001): 'Photoionization of the excited 3s3p $^{1,3}P^0$ states of atomic magnesium.' *J. Phys. B* **34**, 2615–2629. [5]

Kirby, K. P. (1990): 'Molecular photoabsorption processes.' In *Molecular Astrophysics*. Ed. T. W. Hartquist; Cambridge University Press, Cambridge, New York, Port Chester, Melbourne, Sydney, p. 159–180. [5]

Kirby-Docken, K., Liu, B. (1977): 'Theoretical study of molecular dipole moment functions. I. The $X^1\,\Sigma^+$ state of CO*.' *J. Chem. Phys.* **66**, 4309–4316. [5, 10]

Kirby, K. P., van Dishoeck, E. F. (1988): 'Photodissociation processes.' *Adv. Atom. Mol. Phys.* **25**, 437–476. [5]

Kirby, K., Uzer, T., Allison, A. C., Dalgarno, A. (1981): 'Dissociative photoionization of H_2 at 26.9 and 30.5 eV.' *J. Chem. Phys.* **75**, 2820–2825. [5]

Kiss, Z. J., Welsh, H. L. (1959): 'Pressure-induced infrared absorption of mixtures of rare gases.' *Phys. Rev. Lett.* **2**, 166–168. [8]

Kittel, C. (1963): *Quantum Theoy of Solids* John Wiley & Sons, Inc., New York, London. [4]

Kittel, C., Kroemer, H. (1980): *Thermal Physics*. 2^{nd} ed., W. H. Freeman and Co., New York, San Francisco, London. [4]

Kivel, B. (1954): 'Opacity of Air at High Temperatures.' Los Alamos National Laboratory report LA-1738. [1]

Kivel, B. (1967a): 'Neutral atom bremsstrahlung.' *J. Quant. Spectr. Rad. Transfer* **7**, 27–49. [6]

Kivel, B. (1967b): 'Bremsstrahlung in air.' *J. Quant. Spectr. Rad. Transfer* **7**, 51–60. [6]

Kivel, B., Mayer, H., Bethe, H. (1957): 'Radiation from hot air. Part I. Theory of nitric oxide absorption.' *Ann. Phys. (NY)* **2**, 57–80. [1, 7]

Klein, O. (1932): 'Zur Berechnung von Potentialkurven für zweiatomige Moleküle mit Hilfe von Spektraltermen.' *Z. Physik* **76**, 226–235. [3]

Klotz, I. M., Rosenberg, R. M. (2008): *Chemical Thermodynamics, Basic Theory and Methods*. 7^{th} ed., John Wiley & Sons, Inc., Hoboken, N.J. [4]

Kobus, J. (1997): 'Diatomic molecules: Exact solutions of HF equations.' In *Advances in Quantum Chemistry: Recent Advances in Computational Chemsitry*. Eds. P.-O. Lowden, J. R. Sabin, M. C. Zerner, J. Karwowski, M. Karelson; Academic Press, New York, London, p. 2–15. [3]

Koch, H. W., Motz, J. W. (1959): 'Bremsstrahlung cross-section formulas and related data.' *Rev. Mod. Phys.* **31**, 920–955. [5]

Kohn, W., Sham, L. J. (1965): 'Self-consistent equations including exchange and correlation effects.' *Phys. Rev. A* **140**, 1133–1138. [3, 4]

Kong, F.-A. (1982): 'The periodicity of diatomic molecules.' *J. Mol. Struct.* **90**, 17–28. [3]

Koopmans, T. (1934): 'Über die Zuordnung von Wellenfunktionen und Eigenwerten zu den einzelnen Elektronen eines Atoms.' *Physica* **1**, 104–113. [3]

Kourganoff, V. (1963): *Basic Methods in Transfer Problems*. Dover Publication, Inc., New York. [2]

Kovács, I. (1969): *Rotational Structure in the Spectra of Diatomic Molecules*. American Elsevier Publ. Co., New York. [3, 5]

Kovetz, A., Shaviv, G. (1973): 'The electrical and thermal conductivities of stellar degenerate matter.' *Astron. Astrophys.* **28**, 315–318. [9]

Kraeft, W. D., Schlanges, M., Kremp, D. (1986): 'A quantum kinetic equation for nonideal gases in the three-particle collision approximation.' *J. Phys. A* **19**, 3251–3260. [4]

Kraemer, W.-P., Diercksen, G. H. F. (1976): 'Identification of interstellar X-ogen as HCO^+.' *Astrophys. J.* **205**, L97–L100. [3]

Kraemer, W. P., Bunker, P. R., Yoshimine, M. (1984): 'Theoretical study of the rotation–vibration energy levels and dipole moment functions of CCN^+, CNC^+, and C_3.' *J. Mol. Spectr.* **107**, 191–207. [3]

Krainov, V. P., Reiss, H. R., Smirnov, B. M. (1997): *Radiative Processes in Atomic Physics.* Wiley & Sons, New York, Chichester, Weinheim, Brisbane, Singapore, Toronto. [5]

Kramers, H. A. (1923): 'On the theory of x-ray absorption and of the continuous x-ray spectrum.' *London, Edinburgh and Dublin Philos. Mag. J. Sci. Ser. 6* **46**, 836–871. [5]

Kramers, H. A. (1927): 'La diffusion de la lumière par les atomes.' *Atti Congr. Int. Fisico Como-Pavia-Roma* **2**, 545–557. [5]

Krasnikov, Yu. G. (1968): 'Concerning the thermodynamics of a dense plasma.' *Zh. Eksper. Teor. Fiz.* **53**, 2223–2232 (*Sov. Phys. - JETP* **26**, 1252–1256). [4]
Krasnikov, Yu. G. (1977): 'Thermodynamics of nonideal low-temperature plasma.' *Zh. Eksper. Teor. Fiz.* **73**, 516–525 (*Sov. Phys. - JETP* **46**, 270–274). [4]
Krasnikov, Yu. G., Kucerenko, V. I. (1978): 'Thermodynamics of nonideal low-temperature multicomponent plasma: Chemical model.' *High Temp.* **16**, 34–42 (*Teplofizika Vysokikh Temperatur* **16**, 43–53.) [4]
Kronig, R. de L. (1926): 'On the theory of dispersion of x-rays.' *J. Opt. Soc. Am.* **12**, 547–557. [5]
Kronig, R. de L. (1930): *Band Spectra and Molecular Structure*. MacMillan Co., New York; At the University Press, Cambridge, England. [3]
Kronig, R. de L., Kramers, H. A. (1928): 'Zur Theorie der Absorption und Dispersion in den Röntgenspektren.' *Z. Physik* **48**, 174–179. [5]
Krügel, E. (2003): *The Physics of Interstellar Dust*. Institute of Physics and Astrophysics, Bristol, UK. [5]
Krupenie, P. H. (1972): 'The spectrum of molecular oxygen.' *J. Phys. Chem. Ref. Data* **1**, 423–534. [3, 5]
Krupp, B. M., Collins, J. G., Johnson, H. R. (1978): 'The effects of TiO opacity on the atmospheric structure of cool stars.' *Astrophys. J.* **219**, 963–969. [7]
Kubo, R. (1956): 'A general expression for the conductivity tensor.' *Can. J. Phys.* **34**, 1274–1277. [7]
Kubo, R. (1957): 'Statistical-mechanical theory of irreversible processes. I. General theory and simple applications to magnetic and conductive problems.' *J. Phys. Soc. Japan* **12**, 570–586. [7]
Kubo, R. (1959): 'Some aspects of the statistical-mechanical theory of irreversible processes.' In *Lectures in Theoretical Physics*, Vol. 1. Ed. W. E. Britten, L. G. Dunham; Interscience Publishers, Inc., New York, p. 120–203. [5, 8]
Kubo, R. (1962a): 'A stochastic theory of line-shape and relaxation.' In *Fluctuation, Relaxation, and Resonance in Magnetic Systems*. Ed. D. ter Haar; Oliver and Boyd, Edinburg, p. 23–68. [7]
Kubo, R. (1962b): 'Generalized cumulant expansion method.' *J. Phys. Soc. Japan* **17**, 1100–1120. [7]
Kubo, R. (1971): *Statistical Mechanics.* North Holland, Amsterdam. [7]
Kuchitsu, K., Morino, Y. (1965): 'Estimation of anharmonic potential constants. II. Bent XY_2 molecules.' *Bull. Chem. Soc. Japan* **38**, 814–824. [5]
Kuhn, H. G. (1969): *Atomic Spectra*. 2^{nd} ed., Longmans, Green & Co. Ltd., London & Harlow. [5]
Kuntz, M., Höpfner, M. (1999): 'Efficient line-by-line calculation of absorption coefficients.' *J. Quant. Spectr. Rad. Transfer* **63**, 97–114. [7]
Kupka, H., Cribb, P. H. (1986): 'Multidimensional Franck–Condon integrals and Duschinsky mixing effects.' *J. Chem. Phys.* **85**, 1303–1315. [5]
Kurucz, R. L. (1970): 'ATLAS: A computer program for calculating model stellar atmospheres.' Smithsonian Astrophysical Observatory special report 309. [1, 7]
Kurucz, R. L. (1979): 'Model atmospheres for G, F, A, B, and O stars.' *Astrophys. J. Suppl. Ser.* **40**, 1–340. [1, 7]
Kurucz, R. L. (1991): 'New opacity calculations.' In *Stellar Atmospheres: Beyond Classical Models*, Eds. L. Crivellari, I. Hubeny, and D. G. Hummer; Kluwer Academic Publ., p. 441–448. [1, 7]
Kurucz, R. L., Avrett, E. H. (1981): 'Solar spectrum synthesis.' Smithsonian Astrophys. Obs. Special report 391. [7, 10]
Kurucz, R. L., Peytremann, E., Avrett, E. H. (1975): *Blanketed Model Atmospheres for Early-Type Stars.* Smithsonian Institution Press, Washington, DC. [1, 7]
Kuz'menko, N. E., Kuznetsova, L. A., Monyakin, A. P., Kuzyakov, Yu. Ya., Plastinin, Yu. A. (1979): 'Electronic transition probabilities and lifetimes of electronically excited states of diatomic molecules.' *Usp. Fiz. Nauk* **127**, 451–478; Engl. trans. (*Sov. Phys. Usp.* **22**, 160–173). [5]

Kuz'menko, N. E., Kuznetsova, L. A., Monyakin, A. P., Kuzyakov, Yu. Ya. (1980): 'Probabilities for electronic transitions of molecular systems of high-temperature air components – I. The Schumann–Runge system of the O_2-molecule and the first positive system of the N_2-molecule. *J. Quant. Spectr. Rad. Transfer* **24**, 29–41. [5]

Kuznetsova, L. A. (1987): 'Electronic transition strengths for diatomic molecules.' *Spectr. Lett*. **20**, 665–723. [5]

Kuznetsova, L. A., Kuz'menko, N. E., Kuzyakov, Yu. Ya., Plastinin, A. (1974): 'Probabilities of optical transitions in electronic vibration–rotation spectra of diatomic molecules.' *Usp. Fiz. Nauk* **113**, 285–325; Engl. trans. (*Sov. Phys. Usp.* **17**, 405–423). [5]

Labani, B., Bonamy, J., Robert, C., Hartmann, J. M., Taine, J. (1986): 'Collisional broadening of rotation–vibration lines for asymmetric top molecules. I. Theoretical model for both distant and close collisions.' *J. Chem. Phys.* **84**, 4256–4267. [7]

Labzowsky, L. N., Klimchitskaya, G. L., Dmitriev, Yu. Yu. (1993): 'Relativistic effects in the spectra of atomic systems.' Institute of Physics Publishing, Bristol, Philadelphia. [5]

Lacis, A. A., Oinas, V. J. (1991): 'A description of the correlated-k distribution method for modeling nongray gaseous absorption, thermal emission, and multiple scattering in vertically inhomogeneous atmospheres.' *J. Geophys. Res.* **96**, 9027–9063. [7]

Ladenburg, R. (1914): 'Atoms concerned in emission of spectral lines.' *Verhandl. deut. physik. Ges.* **16**, 765–779. [6]

Ladenburg, R. (1921): 'Die quantentheoretische Deutung der Zahl der Dispersionselektronen.' *Z. Physik* **4**, 451–468. [6]

Ladenburg, R., van Voorhis, C. C. (1933): 'The continuous absorption of oxygen between 1750 and 1300 Å and its bearing upon the dispersion.' *Phys. Rev.* **43**, 315–321. [6]

Ladik, J., Cizek, J., Mukherjee, P. K. (1981): 'Relativistic Hartee-Fock theories for molecules and crystals in a linear combination of atomic orbitals form.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 305–334. [3]

Lam, K. S. (1977): 'Application of pressure broadening theory to the calculation of atmospheric oxygen and water vapor microwave absorption.' *J. Quant. Spectr. Rad. Transfer* **17**, 351–383. [7]

Lampe, M. (1968a): 'Transport coefficients of degenerate plasma.' *Phys. Rev.* **170**, 306–319. [9]

Lampe, M. (1968b): 'Transport theory of a partially degenerate plasma.' *Phys. Rev.* **174**, 276–289. [9]

Landshoff, R. (1949): 'Transport phenomena in a completely ionized gas in presence of a magnetic field.' *Phys. Rev.* **76**, 904–909. [9]

Landshoff, R. K. M., Magee, J. L. (Eds.) (1969): *Thermal Radiation Phenomena, Vol. 1: Radiative Properties of Air*. IFI/Plenum Data Corp., Plenum Publ. Corp. New York, Washington. [1]

Langhoff, P. W. (1983a): 'Schrödinger Spectra.' In *Methods in Computational Molecular Physics*. Eds. G. H. F. Diercksen and S. Wilson; D. Reidel, Dordrecht, Boston, p. 299–333. [5]

Langhoff, P. W. (1983b): 'Aspects of electonic configuration interaction in molecular photoionization.' In *Electron–Atom and Electron–Molecule Collisions.* Ed. J. Hinze; Plenum Press, New York, p. 297–313. [5]

Langhoff, P. W. (1988): 'Stieltjes methods for Schrodinger spectra: Hilbert-space approximations to the discrete and continuum eigenstates of spatially anisotropic Hamiltonian operators.' In *Mathematical Frontiers in Computational Chemical Physics.* Ed. D. G. Truhlar; Springer-Verlag, New York, Berlin, Heidelberg, London, Paris, Tokyo, p. 85–135. [5]

Langhoff, P. W., Padial, N., Csanak, G., Rescigno, T. N., McKoy, B. V. (1980): 'Theoretical studies of photoionization in diatomic and polyatomic molecules.' *Int. J. Quantum Chem. Symp.* **14**, 285–304. [5]

Langhoff, S. R., van Dishoeck, E. F., Wetmore, R., Dalgarno, A. (1982): 'Radiative lifetimes and dipole moments of the $A^2\Sigma^+$, $B^2\Sigma^+$, and $C^2\Sigma^+$ states of OH.' *J. Chem. Phys.* **77**, 1379–1390. [5]

Larimer, J. W. (1973): 'Chemistry of the solar nebula.' In *Cosmochemistry*. Ed. A. G. W. Cameron, Astrophys. Space Sci. Lib. **40**, D. Reidel Publ. Co., Dordrecht-Holland, p. 103–120. [4]

Larkin, A. I. (1960): 'Thermodynamic functions of a low-temperature plasma.' *Zh. Eksper. Teor. Fiz.* **38**, 1896–1898 (*Sov. Phys. - JETP* **11**, 1363–1364). [4]

Larsson, M., Siegbahn, P. E. M. (1983): 'A theoretical study of the radiation lifetime of the CH $A^2\Delta$ state.' *J. Chem. Phys.* **79**, 2270–2277. [5]

Lassettre, E. N., Skerbele, A. (1974): 'Generalized oscillator strengths for 7.4 eV excitation of H_2O at 300, 400, and 500 eV kinetic energy. Singlet–triplet energy differences.' *J. Chem. Phys.* **60**, 2464–2469. [5]

Latter, R. (1955): 'Temperature behavior of the Thomas–Fermi statistical model for atoms.' *Phys. Rev.* **99**, 1854–1870. [4]

Lax, M. (1952): 'The Franck–Condon principle and its application to crystals.' *J. Chem. Phys.* **20**, 1752–1760. [7]

Layzer, D. (1959): 'On a screening theory of atomic spectra.' *Ann. Phys. (NY)* **8**, 271–296. [3]

Layzer, D., Bahcall, J. (1962): 'Relativistic Z-dependent theory of many-electron atoms.' *Ann. Phys. (NY)* **17**, 177–204. [3]

Lebedev, V. S., Beigman, I. I. (1998): *Physics of Highly Excited Atoms and Ions*. Springer-Verlag, Berlin, Heidelberg, New York. [5]

Lee, B. I., Kesler, M. G. (1975): 'A generalized thermodynamic correlation based on three-parameter corresponding states.' *Am. Inst. Chem. Eng. J.* **21**, 510–527. [4]

Lee, C. M., Thorsos, E. I. (1978): 'Properties of matter at high pressures and temperatures.' *Phys. Rev. A* **17**, 2073–2076. [4]

Lee, C. M., Kissel, L., Pratt, R. H., Tseng, H. K. (1976): 'Electron bremsstrahlung spectrum, 1–500 keV.' *Phys. Rev. A* **13**, 1714–1727. [5]

Lee, R. W. (1987): 'Very very very simple to use (and accurate) spectral line-broadening codes for hydrogen-, helium- and lithium-like ions in plasmas.' Livermore Lawrence National Laboratory report UCID-21292. [7]

Lee, T. D. (1950): 'Hydrogen content and energy-productive mechanism of white dwarfs.' *Astrophys. J.* **111**, 625–640. [9]

Lefebvre-Brion, H., Field, R. W. (1986): *Perturbations in the Spectra of Diatomic Mmolecules.* Academic Press, Orlando. [5]

Lenard, A. (1960): 'On Bogoliubov's kinetic equation for a spatially homogeneous plasma.' *Ann. Phys. (NY)* **10**, 390–400. [9]

Lengsfield, B. H., Jafri, J. A., Phillips, D. H., Bauschlicher Jr., C. W. (1981): 'On the use of corresponding orbitals in the calculation of nonorthogonal transition moments.' *J. Chem. Phys.* **74**, 6849–6856. [5]

Lenoble, J. (1985): *Radiative Transfer in Scattering and Absorbing Atmospheres: Standard Computational Procedures*. A. Deepak Publishing, Hampton, VA. [2]

Lenoble, J. (1993): *Atmospheric Radiative Transfer*. A. Deepak Publishing, Hampton, VA. [7]

LeRoy, R. J., Macdonald, R. G., Burns, G. (1976): 'Diatom potential curves and transition moment functions from continuum absorption coefficients: Br_2.' *J. Chem. Phys.* **65**, 1485–1500. [7]

Leszczynski, J. (1996): *Computational Chemistry: Reviews of Current Trends.* World Scientific, Singapore, New Jersey, London, Hong Kong, Bangalore, Taipei. [3]

Levi di Leon, R., Taine, J. (1986): 'A fictive gas-method for accurate computation of low-resolution IR gas transmissivities: Application to the 4.3 μm CO_2 band.' *Rev. Phys. App.* **21**, 825–832. [7]

Levine, H. B., Birnbaum, G. (1967): 'Classical theory of collision-induced absorption in rare-gas mixtures.' *Phys. Rev.* **154**, 86–92. [8]

Levine, Z. H., Sovin, P. (1983): 'Electron correlation effects in photoemission from the $1\pi_u$ level in acetylene.' *Phys. Rev. Lett.* **50**, 2074–2077. [5]

Lewis, G. N. (1901a): 'The laws of physico-chemical change.' *Daedalus, Proc. Am. Acad. Arts Sci.* **37**, 49–69. [4]

Lewis, G. N. (1901b): 'Das Gesetz physiko-chemischer Vorgänge.' *Z. Phys. Chem.* **38**, 205–226. [4]

Lewis, M. (1961): 'Stark broadening of spectral lines by high-velocity charged particles.' *Phys. Rev.* **121**, 501–505. [7]

Li, X., Paldus, J. (1997): 'Perturbation theory for low-spin open-shell states.' In *Advances in Quantum Chemistry: Recent Advances in Computational Chemsitry*. Eds. P.-O. Lowden, J. R. Sabin, M. C. Zerner, J. Karwowski, M. Karelson; Academic Press, New York, London, p. 16–33. [3]

Liberman, D. (1962): 'Upper Limits on the Rosseland Mean Opacity.' Los Alamos Scientific Laboratory report LA-2700. [11]

Liberman, D. (1979): 'Self-consistent field model for condensed matter.' *Phys. Rev. B* **20**, 4981–4989. [4]

Liberman, D., Waber, J. T., Cromer, D. T. (1965): 'Self-consistent-field Dirac–Slater wave functions for atoms and ions. I. Comparison with previous calculations.' *Phys. Rev.* **137**, A27–A34. [3]

Liberman, D. A., Cromer, D. T., Waber, J. T. (1971): 'Relativistic self-consistent Field program for atoms and ions.' *Comp. Phys. Comm.* **2**, 107–113. [3]

Lin, C. D. (1977): 'Oscillator strengths of transitions between low-lying S and P states of helium-like ions.' *Astrophys. J.* **217**, 1011–1015. [5]

Lin, S. C., Kivel, B. (1959): 'Slow-electron scattering by atomic oxygen.' *Phys. Rev.* **114**, 1026–1027. [6]

Lind, A. C., Greenberg, J. M. (1966): 'Electromagnetic scattering by obliquely oriented cylinders.' *J. Appl. Phys.* **37**, 3195–3203. [5]

Lindgren, I. (1998): 'Development of atomic many-body theory.' In *Many-Body Atomic Physics*. Eds. J. J. Boyle and M. S. Pindzola; Cambridge University Press, Cambridge, New York, Melbourne, p. 3–38. [3]

Lindhard, J. (1954): 'On the properties of a gas of charged particles.' *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **28**, No. 8. [5]

Lindholm, E., Åsbrink, L. (1985): *Molecular Orbitals and their Energies, Studied by the Semiempirical HAM Method.* Springer-Verlag, Berlin, New York. [3]

Linsky, J. L. (1969): 'On the pressure-induced opacity of molecular hydrogen in late-type stars.' *Astrophys. J.* **156**, 989–1006. [8]

Liu, Z. (1998): 'Direct double photoionization in atoms.' In *Many-Body Atomic Physics*. Eds. J. J. Boyle and M. S. Pindzola; Cambridge University Press, Cambridge, New York, Melbourne, p. 150–156. [5]

Loftus, A., Krupenie, P. H. (1977): 'The spectrum of molecular nitrogen.' *J. Phys. Chem. Ref. Data* **6**, 113–307. [3, 5]

Löwdin, P.-O. (1955): 'Quantum theory of many-particle systems. I. Physical interpretation by means of density matrices, natural spin-orbitals, and convergence problems in the method of configurational interaction.' *Phys. Rev.* **97**, 1474–1489. [3]

Löwdin, P.-O. (1963): 'Studies in perturbation theory. Part I. An elementary iteration-variation procedure for solving the Schrödinger equation by partitioning techniques.' *J. Mol. Spectr.* **10**, 12–33. [5]

Louck, J. C. (1976): 'Derivation of the molecular vibration-rotation Hamiltonian from the Schrödinger equation for the molecular model.' *J. Mol. Spectr.* **61**, 107–137. [3]

Lucas, N. J. D. (1973): 'The Franck–Condon principle for polyatomic molecules.' *J. Phys. B* **6**, 155–163. [5]

Lucchese, R. R., Raseev, G., McKoy, V. (1982): 'Studies of differential and total photoionization cross sections of molecular nitrogen.' *Phys. Rev. A* **25**, 2572–2587. [5]

Lucchese, R. R., Takatsuka, K., Watson, D. K., McKoy, V. (1983): 'The Schwinger variational principle: An approach to electron–molecule collisions.' In *Electron–Atom and Electron–Molecule Collisions.* Ed. J. Hinze; Plenum Press, New York, p. 29–49. [5]

Lucchese, R. R., Zurales, R. W. (1990): 'Comparison of the differential and total photoionization cross sections of N_2 in the multichannel frozen-core Hartree–Fock and random phase approximations.' *Bull. Am. Phys. Soc.* **35**, 1166. [5]

Ludwig, C. B. (1971): 'Measurements of the curves-of-growth of hot water vapor.' *Appl. Optics* **10**, 1057–1073. [13]

Ludwig, C. B., Ferriso, C. C. (1967): 'Prediction of total emissivity of N_2-broadened and self-broadened hot water vapor.' *J. Quant. Spectr. Rad. Transfer* **7**, 7–26. [7, 13]

Ludwig, C. B., Malkmus, W., Reardon, J. E. Thomson, J. A. L. (1973): 'Handbook of infrared radiation from combustion gases.' *NASA report SP-3080*, Washington, DC. [7, 11, 13]

Lukirskii, A. P., Brytov, I. A., Zimkina, T. M. (1964): 'Photoionization absorption of He, Kr, Xe, CH_4, and methylal in the 23.6–250 Å region.' *Optics Spectrosk. (USSR)* **17**, 234–237. [5]

Lundqvist, S., Sjölander, A. (1964): 'On polarization waves in van der Waals crystals.' *Arkiv Fysik* **26**, 17–34. [5]

Luo, D., Pradhan, A. K. (1989): 'Atomic data for opacity calculations: XI. The carbon isoelectronic sequence.' *J. Phys. B* **22**, 3377–3395. [3]

Luzhkov, V., Warshel, A. (1991): 'Microscopic calculations of solvent effects on absorption spectra of conjugated molecules.' *J. Am. Chem. Soc.* **113**, 4491–4499. [5]

Lynch, R. (1995): 'Halfwidths and line shifts of water vapor perturbed by both nitrogen and oxygen.' Ph. D. dissertation, Phys. Dept., U. Massachusetts, Lowell. [7]

Lynch, R., Gamache, R. R., Neshyba, S. P. (1998): 'N_2 and O_2 induced halfwidths and line shifts of water vapor transitions in the (301) ← (000) and (221) ← (000) bands.' *J. Quant. Spectr. Rad. Transfer* **59**, 595–613. [7]

Ma, Q., Tipping, R. H. (1991): 'A far wing line-shape theory and its application to the water continuum absorption in the infrared region.' *J. Chem. Phys.* **95**, 6290–6301. [7]

Ma, Q., Tipping, R. H. (1992a): 'A far wing line-shape theory and its application to the water vibrational bands. (II).' *J. Chem. Phys.* **96**, 8655–8663. [7]

Ma, Q., Tipping, R. H. (1992b): 'A far wing line-shape theory and its application to the foreign-broadened water continuum absorption. III.' *J. Chem. Phys.* **97**, 818–828. [7]

Ma, Q., Tipping, R. H. (1994): 'The detailed balance requirement and general empirical formalisms for continuum absorption.' *J. Quant. Spectr. Rad. Transfer* **51**, 751–757. [7]

Ma, Q., Tipping, R. H., Boulet, C. (1996): 'The frequency detuning and band-average approximations in a far wing line shape theory satisfying detailed balance.' *J. Chem. Phys.* **104**, 9678–9688. [7]

Mackowski, D. W. (1991): 'Analysis of radiative scattering for multiple sphere configurations.' *Proc. Roy. Soc. London Ser. A* **433**, 599–614. [5]

Mackowski, D. W. (1995): 'Calculation of total cross sections of multiple-sphere clusters.' *J. Opt. Soc. Am. A* **11**, 2851–2861. [5]

Madden, R. P., Codling, K. (1963): 'New autoionizing atomic energy levels in He, Ne, and Ar.' *Phys. Rev. Lett.* **10**, 516–518. [5]

Magee, J. L., Aroeste, H. (1967): 'Thermal Radiation Phenomena,' Vol. 1–4. Defense Atomic Support Agency report DASA 1917. [1]

Magee Jr., N. H., Abdallah Jr., J., Clark, R. E. H., Cohen, J. S., Collins, L. A., Csanek, G., Fontes, C. J. Gauger, A., Keady, J. J., Kilcrease, D. P., Merts, A. L. (1995): 'Atomic structure calculations and new Los Alamos astrophysical opacities.' In *Astrophysical Applications of Powerful New Databases: Joint Discussion no. 16 of the 22nd General Assembly of the IAU.* Eds. S. J. Adelman, W. L. Wiese, Astronomical Society of the Pacific Conference Series, **78** San Francisco. [13]

Mahan, G. D., Subbaswamy, K. R. (1990): *Local Density Theory of Polarizability*. Plenum Press, New York, London. [7]

Mahapatra, S. (2002): 'Unraveling the highly overlapping $\tilde{A}^2B_2$, $\tilde{B}^1A_1$, photoelectron bands of Cl_2O: Nonadiabatic effects due to conical interactions.' *J. Chem. Phys.* **116**, 8817–8826. [5]

Malkmus, W. (1963): 'Infrared emissivity of carbon dioxide (4.3-μm band).' *J. Opt. Soc. Am.* **53**, 951–961. [7]

Malkmus, W. (1967): 'Random Lorentz band model with exponential-tailed S^{-1} line-intensity distribution function.' *J. Opt. Soc. Am.* **57**, 323–329. [7]

Malkmus, W. (1968): 'Random band models with lines of pure Doppler shape.' *J. Opt. Soc. Am.* **58**, 1214–1217. [7]

Malkmus, W., Thomson, A. (1961): 'Infrared emissivity of diatomic gases for the anharmonic vibrating-rotator model.' *J. Quant. Spectr. Rad. Transfer* **2**, 17–39. [7]

Mallard, W. G., Westley, F., Herron, J. T., Hampson, R. F., Frizzell, D. H. (1998): 'NIST Standard Reference Database 17.' *NIST Chemical Kinetics Database* U.S. Dep. of Commerce, Technology Administration, National Institute of Standards and Technology, Stand. Ref. Data, Gaithersburg, MD 20899. [4]

Malli, G. L. (1981): 'Relativistic self-consistent-field theory for molecules.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 183–212. [3]

Mann, J. B. (1967): 'Atomic Structure Calculations, I. Hartree–Fock Energy Results for the Elements Hydrogen to Lawrencium.' Los Alamos Scientific Laboratory report LA-3690. [3, 4]

Mann, J. B. (1968): 'Atomic Structure Calculations, II. Hartree–Fock Wavefunctions and Radial Expectation Values: Hydrogen to Lawrencium.' Los Alamos Scientific Laboratory report LA-3691. [3]

Mann, J. B., Waber, J. T. (1970): 'SCF relativistic Hartree–Fock calculations on the superheavy elements 118–131.' *J. Chem. Phys.* **53**, 2397–2406. [3]

Manneback, C. (1951): 'Computation of the intensities of vibrational spectra of electronic bands in diatomic molecules.' *Physica* **17**, 1001–1010. [5]

Manson, S. T., Kennedy, D. J. (1974): 'X-ray emission rates in the Hartree–Slater approximation.' *Atomic Data Nucl. Data Tables* **14**, 111–120. [5]

Mantz, A. W., Watson, J. K. G., Narahari Rao, K., Albritton, D. L., Schmeltekopf, A. L., Zare, R. N. (1971): 'Rydberg–Klein–Rees potential for the $X\,^1\Sigma^+$ state of the CO molecule.' *J. Mol. Spectr.* **39**, 180–184. [5]

Margenau, H. (1939): 'Van der Waals forces.' *Rev. Mod. Phys.* **11**, 1–35. [7]

Margenau, H., Watson, W. W. (1936): 'Pressure effects on spectral lines.' *Rev. Mod. Phys.* **8**, 22–53. [7]

Marić, D., Burrows, J. P. (1996): 'Application of a Gaussian distribution function to describe molecular UV-visible absorption continua.' *J. Phys. Chem.* **100**, 8645–8659. [7]

Marić, D., Burrows, J. P. (1999): 'Analysis of UV absorption spectrum of ClO: A comparative study of four methods for spectral computation.' *J. Quant. Spectr. Rad. Transfer* **62**, 345–369. [7]

Marin, O., Buckius, R. O. (1998): 'A model of the cumulative distribution function for wide band radiative properties.' *J. Quant. Spectr. Rad. Transfer* **59**, 671–685. [7]

Marques, M. A. L., Marques, C. A., Nogueira, F., Rubio, A., Burke, K., Gross, E. K. U. (2006): *Time-Dependent Density Functional Theory*, Series Lecture Notes in Physics **706**, Springer-Verlag. [3]

Marr, G. V. (1967): *Photoionization Processes in Gases*. Academic Press, New York, London. [1]

Marr, G. V., Morton, J. M., Holmes, R. M., McCoy, D. G. (1979): 'Angular distribution of photoelectrons from free molecules of N_2 and CO as a function of photon energy.' *J. Phys. B* **12**, 43–52. [5]

Marshak, R. E. (1945): 'Opacity of Air, BeO, C, Fe, and U at High Temperatures.' Los Alamos National Laboratory report LA-229. [1]

Marshall, W. (1960): 'The kinetic theory of an ionized gas.' UK Atomic Energy Authority report AWRE T/R 2247, Part 2: 2352, Part 3: 2419, Harwell, Berkshire, England. [9]

Martin, G. A., Fuhr, J. R., Wiese, W. L. (1988): 'Atomic transition probabilities scandium through manganese.' *J. Phys. Chem. Ref. Data* (Suppl. 3) **17**, 1–523. [5]

Martin, P. C., Schwinger, J. (1959): 'Theory of many-particle systems. I.' *Phys. Rev.* **115**, 1342–1373. [4]

Martin, W. C., Zalabas, R., Hagan, L. (1978): *Atomic Energy Levels.* Natl. Stand. Ref. Data Ser. National Bureau of Standards, 60. [3, 4]

Matsubara, T. (1955): 'A new approach to quantum-statistical mechanics.' *Prog. Theor. Phys.* **14**, 351–378. [4]

Mayer, H. (1947): 'Methods of Opacity Calculations.' Los Alamos Scientific Laboratory report LA-647. [1, 2, 3, 4, 7, 11]

Mayer, H. L., (Ed.) (1964): 'Conference on opacities.' *J. Quant. Spectr. Rad. Transfer* **4**, 581–760. [1, 13]

Mayer, J. E., Mayer, M. G. (1940): *Statistical Mechanics.* J. Wiley & Sons, New York. [7]
McCallum, J. C. (1979): 'Computational study of the accuracy of the r-centroid approximation.' *J. Quant. Spectr. Rad. Transfer* **21**, 563–572. [5]
McCurdy Jr., C. W., Rescigno, T. N., Yeager, D. L., McKoy, V. (1977): 'The equations of motion method: An approach to the dynamical properties of atoms and molecules.' In *Methods of Electronic Structure Theory.* Ed. H. F. Schaefer, III; Plenum Press, New York, London, p. 339–386. [5]
McDougall, J., Stoner, E. C. (1938): 'The computation of Fermi–Dirac functions.' *Phil. Trans. Roy. Soc. London, Ser. A* **237**, 67–104. [4, 9]
McGuire, E. J. (1968): 'Photo-ionization cross sections of the elements helium to xenon.' *Phys. Rev.* **175**, 20–30. [5]
McQuarrie, D. A. (1976): *Statistical Mechanics.* Harper and Row Publishers, New York, Evanston, San Francsco, London. [5, 7]
McWeeny, R. (1992): 'The electron correlation problem.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 47–56. [3]
Mebel, A. M., Hayashi, M., Liang, K. K., Lin, S. H. (1999): 'Ab initio calculations of vibronic spectra and dynamics for small polyatomic molecules: Role of Duschinsky effect.' *J. Phys. Chem. A* **103**, 10674–10690. [5, 7]
Meerts, W. L., Dymanus, A. (1973): 'Electric dipole moments of OH and OD by molecular beam electric resonance.' *Chem. Phys. Lett.* **23**, 45–47. [5]
Meggers, W. F., Corliss, C. H., Scribner, B. F. (1975): *Tables of Spectral Line Intensities.* NBS Monograph 145, Part I, U. S. Government Printing Office, Washington, DC. [5]
Mendoza, C. (1992): 'Atomic data from the opacity project.' In *Atomic and Molecular Data for Space Astronomy – Needs, Analysis, and Availability*. Eds. P. L. Smith, W. L. Wiese; Springer-Verlag, Berlin, Heidelberg, New York, London, Paris, Tokyo, Hong Kong, Barcelona, Budapest, p. 85–119. [3, 10]
Menzel, D. H. (1968): 'Oscillator strengths for high-level transitions in H.' *Nature* **218**, 756–757. [5]
Menzel, D. H. (1969): 'Oscillator strengths, f, for high-level transitions in hydrogen.' *Astrophys. J. Suppl. Ser.* **18**, 221–246. [5]
Menzel, D. H., Goldberg, L. (1936): 'Multiplet strengths for transitions involving equivalent electrons.' *Astrophys. J.* **84**, 1–10. [5]
Menzel, D. H., Pekeris, C. L. (1936): 'Absorption coefficients and hydrogen line intensities.' *Mon. Not. Roy. Astron. Soc.* **96**, 77–111. [5]
Menzel, D. H., Bhatnagar, P. L., Sen, H. K. (1963): *Stellar Interiors*. Chapman & Hall, London. [1]
Mercier, R. P. (1964): 'The radio-frequency emission coefficient of a hot plasma.' *Proc. Phys. Soc. (London)* **83**, 819–822. [6]
Merdji, H, Mißalla, T., Gilleron, F., Chenais-Popovics, C., Gauthier, J. C., Renaudin, P., Gary, S., Bruneau, J. (1997): 'Opacity measurements of a radiatively heated boron sample.' *J. Quant. Spectr. Rad. Transfer* **58**, 783–789. [13]
Merts, A. L., Magee Jr., N. H. (1972): 'On the contribution of autoionization lines to stellar opacities.' *Astrophys. J.* **177**, 137–143. [5, 12]
Mestel, L. (1950): 'On the thermal conductivity in dense stars.' *Proc. Cambridge Phil. Soc.* **46**, 331–338. [9]
Meyer, W. (1976): 'Theory of self-consistent electron pairs. An iterative method for correlated many-electron wavefunctions.' *J. Chem. Phys.* **64**, 2901–2907. [5]
Meyer, W., Borysow, A., Frommhold, L. (1989): 'Absorption spectra of H_2 – H_2 pairs in the fundamental band.' *Phys. Rev. A* **40**, 6931–6949. [8]
Meyerott, R. E., Sokoloff, J., Nicholls, R. W. (1959): 'Absorption Coefficients of Air.' Lockheed Aircraft Corp. Missile and Space Div. Report LMSD-288052, Palo Alto. [7]
Michels, H. H. (1972): 'Theoretical Determination of Electronic Transition Probabilities for Diatomic Molecules.' Air Force Weapons Laboratory report AFWL-TR-72-1. [3]

Mie, G. (1908): 'Beiträge zur Optik trüber Medien speziell kolloidaler Metallösungen.' *Ann. Physik* **25**, 377–445. [5]

Mihalas, D. (1978): *Stellar Atmospheres*. 2^{nd} ed., W. H. Freeman & Co., San Francisco. [1, 2]

Mihalas, D., Mihalas, B. W. (1984): *Foundations of Radiation Hydrodynamics*. Oxford University Press, New York, Oxford. [2]

Mihalas, D., Däppen, W., Hummer, D. G. (1988): 'The equation of state for stellar envelopes. II. Algorithm and selected results.' *Astrophys. J.* **331**, 815–825. [4]

Miller, M. S., McQuarrie, D. A., Birnbaum, G., Poll, J. D. (1972): 'Constant acceleration approximation in collision-induced absorption.' *J. Chem. Phys.* **57**, 618–624. [8]

Mínguez, E., Serrano, J. F., Gámez, M. L. (1988): 'Analysis if atomic models for the extinction coefficient calculation.' *Laser Particle Beams* **6**, 265–275. [13]

Mirone, A., Gauthier, J. C., Gilleron, F., Chenais-Popovics, C. (1997): 'Non-LTE opacity calculations with $n - l$ splitting for radiative hydrodynamic codes.' *J. Quant. Spectr. Rad. Transfer* **58**, 791–802. [13]

Mishchenko, M. I., Hovenier, J. W., Travis, L. D. (2000): *Light Scattering by Nonspherical Particles. Theory, Measurements, and Applications*. Academic Press San Diego, San Francisco, New York, Boston, London, Sydney, Tokyo. [5]

Mitake, S., Ichimaru, S., Itoh, N. (1984): 'Electrical and thermal conductivities of dense matter in the liquid metal phase. II. Low-temperature quantum corrections.' *Astrophys. J.* **277**, 375–378. [9]

Mjolsness, R. C., Ruppel, H. M. (1967a): 'Bremsstrahlung emission from low-energy electrons on atoms.' *Phys. Rev.* **154**, 98–109. [5, 6]

Mjolsness, R. C., Ruppel, H. M. (1967b): 'Contributions of inverse neutral bremsstrahlung to the absorption coefficient of heated air.' *J. Quant. Spectr. Rad. Transfer* **7**, 423–427. [5, 6]

Mjolsness, R. C., Ruppel, H. M. (1969): 'Evaluation of electron – atom bremsstrahlung from elastic scattering.' *Phys. Rev.* **186**, 83–88. [6]

Møller, C., Plesset, M. S. (1934): 'Note on an approximation treatment for many-electron systems.' *Phys. Rev.* **46**, 618–622. [3]

Mok, D. K. W., Lee, E. P. F., Chau, F.-T., Wang, D. C., Dyke, J. M. (2000): 'A new method of calculation of Franck–Condon factors which includes allowance for anharmonicity and the Duschinsky effect: Simulation of the He I photoelectron spectrum of ClO_2.' *J. Chm. Phys.* **113**, 5791–5803. [5]

Moore, C. E. (1949): *Atomic Energy Levels*. Vol. I. National Bureau of Standards, Circ. 467. [3, 4]

Moore, C. E. (1952): *Atomic Energy Levels*. Vol. II. National Bureau of Standards, Circ. 467. [3, 4]

Moore, C. E. (1958): *Atomic Energy Levels*. Vol. III. National Bureau of Standards, Circ. 467. [3, 4]

Moore, C. E. (1968): *An Ultraviolet Multiplet Table*. National Bureau of Standards, Circ. 488, Sect. 1–5. [5]

Moore, C. E. (1971): *Atomic Energy Levels*. Vol. IV National Bureau of Standards, Circ. 467. [3, 4, 5]

Moore, C. E. (1972): 'Selected tables of atomic spectra, atomic energy levels, and multiplet tables. H, D, T' National Bureau of Standards Reference Data Ser. **40** [5]

Moore, C. E., Gallagher, J. W. (1993): *Tables of Spectra of Hydrogen, Carbon, Nitrogen, and Oxygen Atoms and Ions.* Ed. J. W. Gallagher; CRC Press, Boca Raton. [3, 4]

Moores, D. L. (1966): 'Quantum defect theory. IV. The absorption of radiation by calcium atoms.' *Proc. Phys. Soc. (London)* **88**, 843–859. [3]

Moraldi, M., Borysow, A., Frommhold, L. (1988): 'Rotovibrational collision-induced absorption by nonpolar gases and mixtures (H_2-He pairs): Symmetry of line profiles.' *Phys. Rev. A* **38**, 1839–1847. [8]

More, R. M., Skupsky, S. (1976): 'Nuclear motion corrections to the Thomas–Fermi equation of state for high-density matter.' *Phys. Rev. A* **14**, 474–479. [4]

More, R. M., Warren, K. H. (1991): 'Semicalssical calculation of matrix elements.' *Ann. Phys.* **207**, 282–342. [5]

Mori, K., Wiese, W. L., Shirai, T., Nakai, Y., Ozama, K. (1986): 'Spectral data and Grotrian diagrams for highly ionized titanium, Ti V – XXII.' *Atomic Data Nucl. Data Tables* **34**, 79–184. [5]

Morris, J. C., Krey, R. U., Garrison, R. L. (1969): 'Bremsstrahlung and recombination radiation of neutral and ionized nitrogen.' *Phys. Rev.* **180**, 167–183. [13]

Morse, P., Feshbach, H. (1953): *Methods of Theoretical Physics*. McGraw-Hill Book Co., Inc., New York, Toronto, London. [5]

Morton, D. C. (1970): 'The Effective Temperatures of the O Stars.' In *International Astronomical Union Symposium No. 36, Ultraviolet Stellar Spectra and Related Ground-Based Observations*. Eds. L. Houziaux, H. E. Butler; D. Reidel Publ. Co., Dordrecht-Holland. [7]

Moszkowski, S. A. (1962): 'On the energy distribution of terms and line arrays in atomic spectra.' *Prog. Theor. Phys.* **28**, 1–23. [7]

Motte-Tollet, F., Delwiche, J., Heinesch, J., Hubin-Franskin, M. J., Gingell, J. M., Jones, N. C., Mason, N. J., Marston, G. (1998): 'On the high-resolution HeI photoelectron spectrum of Cl_2O.' *Chem. Phys. Lett.* **284**, 452–458. [5]

Mozer, B. (1960): 'Atomic Line Shapes from a Plasma.' Ph. D. Dissertation, Carnegie Institute of Technology, report 3. [7]

Mozer, B., Baranger, M. (1960): 'Electric field distributions in an ionized gas. II.' *Phys. Rev.* **118**, 626–631. [7]

Muchmore, D., Kurucz, R. L., Ulmschneider, P. (1988): 'Effects of CO molecules on the outer solar atmosphere. Dynamical models with opacity distribution functions.' *Astron. Astrophys.* **201**, 138–142. [7]

Müller, T., Vaccaro, P. H., Pérez-Bernal, F., Iachello, F. (1999): 'The vibronically-resolved emission spectrum of disulfur monoxide (S_2O): An algebraic calculation and quantitative interpretation of Franck–Condon transition intensities.' *J. Chem. Phys.* **111**, 5038–5055. [5]

Muenter, J. S. (1975): 'Electric dipole moment of CO.' *J. Mol. Spectr.* **55**, 490–491. [5]

Mukai, S., Mukai, T., Giese, R. H. (1980): 'Scattering of radiation by a large particle with a rough surface.' In *Light Scattering by Irregularly Shaped Particles*, Ed. D. W. Schuerman, Plenum Press, New York, London, p. 219–225. [5]

Mulliken, R. S., Ermler, W. C. (1977): *Diatomic Molecules: Results of Ab Initio Calculations.* Academic Press, New York, San Francisco, London. [3, 5]

Mulliken, R. S., Ermler, W. C. (1981): *Polyatomic Molecules: Results of ab Initio Calculations.* Academic Press, New York, London, Toronto, Sydney, San Francisco. [3, 5]

Murrell, J. N., Carter, S., Farantos, S. C., Huxley, P., Varandas, A. J. C. (1984): *Molecular Potential Energy Functions.* John Wiley & Sons, Chichester, New York, Brisbane, Toronto, Singapore. [3]

Mutschlecner, J. P., Keller, C. F. (1970): 'Semi-empirical solar line blanketing. I. Statistical Basis and Method.' *Solar Phys.* **14**, 294–309. [7]

Mutschlecner, J. P., Keller, C. F. (1972): 'Semi-empirical solar line blanketing. II. The results of blanketing in solar model atmospheres.' *Solar Phys.* **22**, 70–87. [7]

Nahar, S. N., Pradhan, A. K. (1997): 'Electron-ion recombination rate coefficients, photoionization cross sections, and ionization fractions for astrophysically abundant elements. I. C and N.' *Astrophys. J. Suppl. Ser.* **111**, 339–355. [5]

Nakagawa, M., Kohyama, Y., Itoh, N. (1987): 'Relativistic free–free Gaunt factor of the dense high-temperature stellar plasma.' *Astrophys. J. Suppl. Ser.* **63**, 661–684. [6]

Nandkumar, R., Pethick, C. J. (1984): 'Transport coefficients of dense matter in the liquid metal regime.' *Mon. Not. Roy. Astron. Soc.* **209**, 511–524. [9]

National Bureau of Standards (1949): *Tables of Scattering Functions for Spherical Particles*. NBS Applied Mathematics Series **4**, Government Printing Office, Washington. [5]

Neshyba, S. P., Lynch, R., Gamache, R., Gabard, T., Champion, J.-P. (1994): 'Pressure-induced widths and shifts for the ν_3 band of methane.' *J. Chem. Phys.* **101**, 9412–9421. [7]

Neuforge-Verheecke, C., Guzik, J. A., Keady, J. J., Magee Jr., N. H., Bradley, P. A., Noels, A. (2001): 'Helioseismic tests of the new Los Alamos LEDCOP opacities.' *Astrophys. J.* **561**, 450–454. [13]

Nicholls, R. W. (1964): 'Transition probabilities of aeronomically important spectra.' *Annales Géophys*. **20**, 144–181. [5]
Nicholls, R. W. (1977): 'Transition probability data for molecules of astrophysical interest.' *Ann. Rev. Astron. Astrphys.* **15**, 197–234. [5]
Nicholls, R. W., Jarmain, W. R. (1956): 'r-centroids: Average internuclear separations associated with molecular bands.' *Proc. Phys. Soc. (London) A* **69**, 253–264. [5]
Nicholls, R. W., Stewart, A. L. (1962): 'Allowed Transitions.' In *Atomic and Molecular Processes*. Ed. D. R. Bates; Academic Press, New York, London. [3, 5]
Nicolaides, C. A. (1984): 'State-specific theory of electron correlation in excited states.' In *Advanced Theories and Computational Approaches to the Electronic Structure of Molecules*. Ed. C. E. Dykstra; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster, p. 161–184. [5]
Nicolaides, C. A., Beck, D. R. (1978): 'Time dependence, complex scaling, and the calculation of resonances in many-electron systems.' *Int. J. Quantum Chem.* **14**, 457–703. [5]
Nicolaides, C. A., Theodorakopoulos, G. (1980): 'FOTOS applied to molecules: Oscillator strengths in H_2O.' *Int. J. Quantum Chem. Symp*. **14**, 315–322. [5]
Nielson, H. H. (1951): 'The vibration–rotation energies of molecules.' *Rev. Mod. Phys.* **23**, 90–136. [5]
Nielson, H. H. (1959): 'The vibration–rotation energies of molecules and their spectra in the infrared.' In *Handbuch der Physik* XXXVII/1. Ed. S. Flügge; Springer-Verlag, Berlin, Göttingen, Heidelberg. [7]
Noci, G. (1971): 'Atomic processes in the solar corona.' In *Physics of the Solar Corona.* Ed. C. J. Macris; D. Reidel Publ. Co., Dordrecht-Holland, p. 13–28. [4]
Normand, C. E. (1930): 'The absorption coefficient for slow electrons in gases.' *Phys. Rev.* **35**, 1217–1225. [6]
Nozawa, S., Itoh, N., Kohyama, Y. (1998): 'Relativistic thermal bremsstrahlung Gaunt factor for the intracluster plasma.' Astrophys. J. **507**, 530–557. [6]
Nozières, R., Pines, D. (1958): 'Correlation energy of a free electron gas.' *Phys. Rev.* **111**, 442–454. [4]
Numerov, B. (1932): 'Anwendung der Extrapolationsmethode auf die numerische Integration linearer Differentialgleichungen zweiter Ordnung.' *Izvest. Akad. Nauk (SSSR)* **1932**, 1–8. [3]
Nussbaumer, H., Storey, P. J. (1978): '[Fe VI] emission under nebular conditions.' *Astron. Astrophys.* **70**, 37–42. [3]
Oddershede, J. (1978): 'Polarization propagator calculations.' *Adv. Quantum Chem.* **11**, 275–352. [5]
Oddershede, J. (1983): 'Introductory polarization propagator theory.' In *Methods in Computational Molecular Physics*. Eds. G. H. F. Diercksen and S. Wilson; D. Reidel, Dordrecht, Boston, p. 249–271. [5]
Oddershede, J. (1985): 'Calculation of radiative lifetimes of allowed and forbidden transitions,' In *Molecular Astrophysics: State of the Art and Future Directions*. Eds. G. H. F. Diercksen, W. F. Huebner, and P. W. Langhoff; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster, p. 533–547. [5]
Oddershede, J. (1987): 'Propagator methods.' *Adv. Chem. Phys.* **69**, 201–239. [5]
Oddershede, J. (1992): 'Response and propagator methods.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 303–324. [5]
Oddershede, J., Joergensen, P., Yeager, D. L. (1984): 'Polarization propagator methods in atomic and molecular calculations.' *Comp. Phys. Rep.* **2**, 33–92. [5]
Oddershede, J., Gruener, N. E., Diercksen, G. H. F. (1985): 'Comparison between equation of motion and polarization propagator calculations.' *Chem. Phys.* **97**, 303–310. [5]
Oellrich, L., Plöcker, U., Prausnitz, J. M., Knapp, H. (1981): 'Equation-of-state methods for computing phase equilibria and enthalpies.' *Int. Chem. Eng.* **21**, 1–16. [4]
Oertel, G. K., Shomo, L. R. (1968): 'Tables for the calculation of radial multipole matrix elements by the Coulomb approximation.' *Astrophys. J. Suppl. Ser.* **16**, 175–218. [5]

Özkan, I. (1990): 'F–C principle for polyatomic molecules: Axis-switching effects and transformation of normal coordinates.' *J. Molec. Spectr.* **139**, 147–162. [5]

Ogata, S., Ichimaru, S. (1987): 'Critical examination of N dependence in the Monte Carlo calculations for a classical one-component plasma.' *Phys. Rev. A* **36**, 5451–5454. [9]

Ohno, K., Morokuma, K. (1982): *Quantum chemistry literature data base. Bibliography of ab initio calculations for 1978–1980.* Elsevier, Amsterdam. [3, 5]

Ohno, K., Morokuma, K., Hirota, F., Hosoya, H., Iwata, S., Kashiwagi, H., Obara, S., Osamura, Y., Yamamoto, S., Kosugi, N., Nishimoto, K., Tanaka, K., Togasi, M., Yamabe, S. (1982): 'Quantum chemistry literature data base. Supplement 1. Bibliography of ab initio calculations for 1981.' *J. Mol. Struct.* **91**; *THEOCHEM* **8**, 1–252. [3, 5]

Ohno, K., Morokuma, K., Hirota, F., Hosoya, H., Iwata, S., Osamura, Y., Kashiwagi, H., Yamamoto, S., Kosugi, N., Nakatsuji, H., Nishimoto, K., Obara, S., Tanaka, K., Togasi, M., Yamabe, S. (1983): 'Quantum chemistry literature data base. Bibliography of ab initio calculations for 1982.' *J. Mol. Struct.* **106**; *THEOCHEM* **15**, 1–215. [3, 5]

Ohno, K., Morokuma, K., Hirota, F., Hosoya, H., Iwata, S., Osamura, Y., Kashiwagi, H., Yamamoto, S., Kosugi, N., Nakatsuji, H., Nishimoto, K., Obara, S., Tanaka, K., Togasi, M., Yamabe, S. (1984): 'Quantum chemistry literature data base. Bibliography of ab initio calculations for 1983.' *J. Mol. Struct.* **119**; *THEOCHEM* **20**, 1–229. [3, 5]

Ohno, K., Morokuma, K., Hirota, F., Hosoya, H., Iwata, S., Osamura, Y., Kashiwagi, H., Yamamoto, S., Kitaura, K., Kosugi, N., Nakatsuji, H., Obara, S., Tanaka, K., Togasi, M., Yamabe, S. (1985): 'Quantum chemistry literature data base. Supplement 4. Bibliography of ab initio calculations for 1984.' *J. Mol. Struct.* **134**; *THEOCHEM* **27**, 1–298. [3, 5]

Ohno, K., Morokuma, K., Hirota, F., Hosoya, H., Iwata, S., Kashiwagi, H., Yamamoto, S., Kitaura, K., Kosugi, N., Nakatsuji, H., Obara, S., Tanaka, K., Togasi, M., Yamabe, S. (1986): 'Quantum chemistry literature data base. Supplement 5. Bibliography of ab initio calculations for 1985.' *J. Mol. Struct.* **148**; *THEOCHEM* **33**, 181–500. [3, 5]

Ohno, K., Morokuma, K., Hirota, F., Hosoya, H., Iwata, S., Osamura, Y., Kashiwagi, H., Yamamoto, S., Kitaura, K., Kosugi, N., Nakatsuji, H., Obara, S., Tanaka, K., Togasi, M., Yamabe, S. (1987): 'Quantum chemistry literature data base. Supplement 6. Bibliography of ab initio calculations for 1986.' *J. Mol. Struct.* **154**; *THEOCHEM* **39**, 1–315. [3, 5]

Ohno, K., Morokuma, K., Hosoya, H., Hirota, F., Iwata, S., Osamura, Y., Kashiwagi, H., Yamamoto, S., Kitaura, K., Nakatsuji, H., Obara, S., Tanaka, K., Togasi, M., Yamabe, S. (1988): 'Quantum chemistry literature data base. Supplement 7. Bibliography of ab initio calculations for 1987.' *J. Mol. Struct.* **182**; *THEOCHEM* **51**, 1–310. [3, 5]

Oka, T. (1973): 'Collision-induced transitions between rotational levels.' *Adv. Atom. Mol. Phys.* **9**, 127–206. [7]

Omidvar, K., Guimaraes, P. T. (1990): 'New tabulation of the bound–continuum optical oscillator strength in hydrogenic atoms.' *Astrophys. J. Suppl. Ser.* **73**, 555–602. [5]

Omidvar, K., McAllister, A. M. (1995): 'Evaluation of high-level bound–bound and bound–continuum hydrogenic oscillator strengths by asymptotic expansion.' *phys. Rev* A **51**, 1063–1066. [5]

O'Neil, S. V., Reinhardt, W. P. (1978): 'Photoionization of molecular hydrogen.' *J. Chem. Phys.* **69**, 2126–2142. [5]

Onsager, L., (1931a): 'Reciprocal relations in irreversible processes, I.' *Phys. Rev.* **37**, 405–426. [9]

Onsager, L., (1931b): 'Reciprocal relations in irreversible processes, II.' *Phys. Rev.* **38**, 2265–2279. [9]

Ornstein, L. S., Burger, H. C. (1924): 'Strahlungsgesetz und Intesität von Mehrfachlinien.' *Z. Phys.* **24**, 41–47. [5]

O'Rourke, R. C. (1953): 'Absorption of light by trapped electrons.' *Phys. Rev.* **91**, 265–270. [7]

Oster, L. (1961): 'Emission, absorption, and conductivity of a fully ionized gas at radio frequencies.' *Rev. Mod. Phys.* **33**, 525–543. [6, 9]

Oster, L. (1970): 'The free-free emission and absorption coefficients in the radio frequency range at very low temperatures.' *Astron. Astrophys.* **9**, 318–320. [6]

Paldus, J. (1992a): 'Unitary group approach in the many-electron correlation problem.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 57–64. [3]

Paldus, J. (1992b): 'Coupled cluster theory.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 99–194. [3]

Panofsky, W. K. H., Phillips, M. (1962): *Classical Electricity and Magnetism*. 2^{nd} ed., Addison-Wesley, New York. [5]

Papoušek, D., Aliev, M. R. (1982): *Molecular Vibrational-Rotational Spectra: Theory and Applications of High Resolution Infrared, Microwave, and Raman Spectroscopy of Polyatomic Molecules.* Elsevier Scientific Publ. Co., Amsterdam, Oxford, New York. [3]

Parks, D. E., Rotenberg, M. (1972): 'Incoherent x-ray scattering by a statistical atom.' *Phys. Rev. A* **5**, 521–526. [5]

Parks, D. E., Lane, G., Stewart, J. C., Peyton, S. (1968): *Optical Constants of Uranium Plasma*. NASA report NASA-CR-72348. [5, 7]

Patch, R. W. (1971): 'Absorption coefficients for pressure-induced H_2-H_2 vibrational absorption in the fundamental region.' *J. Quant. Spectr. Rad. Transfer* **11**, 1331–1353. [8]

Patch, R. W., Shackleford, W. L., Penner, S. S. (1962): 'Approximate spectral absorption coefficient calculations for electronic band systems belonging to diatomic molecules.' *J. Quant. Spectr. Rad. Transfer* **2**, 263–271. [7]

Paulsen, D. E., Sheridan, W. F., Huffman, R. E. (1970): 'Thermal recombination emission of NO_2.' *J. Chem. Phys.* **53**, 647–658. [5]

Peach, G. (1965): 'A general formula for the calculation of absorption cross sections for free-free transitions in the field of positive ions.' *Mon. Not. Roy. Astron. Soc.* **130**, 361–377. [5]

Peach, G. (1967): 'A revised general formula for the calculation of atomic photoionization cross sections.' *Mem. R. Astr. Soc.* 71, 13–45. [5, 12]

Peach, G. (1970): 'Continuous absorption coefficients for non-hydrogenic atoms.' *Mem. R. Astr. Soc.* 73, 1–123. [5, 12]

Peach, G., Saraph, H. E., Seaton, M. J. (1988): 'Atomic data for opacity calculations: IX. The lithium isoelectronic sequence.' *J. Phys. B* **21**, 3669–3683. [3]

Peacock, N. J., Hobby, M. G., Galanti, M. (1973): 'Satellite spectra for helium-like ions in laser-produced plasmas.' *J. Phys. B* **6**, L298–L304. [13]

Pegg, D. L. (1996): 'Photodetachment.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 681–689. [5]

Peng, D.-Y., Robinson, D. B. (1976): 'New two-constant equation of state.' *Ind. Eng. Chem. Fundam.* **15**, 59–64. [4]

Penner, S. S. (1959): *Quantitative Molecular Spectroscopy and Gas Emissivities*. Addison-Wesley Publ. Co., Reading, Massachusetts, USA. [5, 7, 11]

Penner, S. S., Thomson, A. (1957): 'Infrared emissivities and absorptivities of gases.' J. Appl. Phys. **28**, 614–623. [11]

Penner, S. S., Gray, L. D. (1961): 'Approximate IR emissivity calculations for HCl at elevated temperatures.' *j. Opt. Soc. Am.* **51**, 460–462. [7]

Penner, S. S., Olfe, D. B. (1968): *Radiation and Reentry*. Academic Press, New York, London. [1, 2, 7, 11, 13]

Penner, S. S., Varanasi, P. (1964): 'Approximate band absorption and total emissivity calculations for CO_2.' *J. Quant. Spectr. Rad. Transfer* **4**, 799–806. [7]

Penner, S. S., Varanasi, P. (1965): 'Approximate band absorption and total emissivity calculations for H_2O.' *J. Quant. Spectr. Rad. Transfer* **5**, 391–401. [7, 11, 13]

Penner, S. S., Varanasi, P. (1966): 'Effect of (partial) overlapping of spectral lines on the total emissivity of H_2O-CO_2 mixtures ($T \approx> 800^o$ K).' *J. Quant. Spectr. Rad. Transfer* **6**, 181–192. [13]

Penner, S. S., Varanasi, P. (1967): 'Spectral absorption coefficient in the pure rotation spectrum of water vapor.' *J. Quant. Spectr. Rad. Transfer* **7**, 687–690. [7]

Penner, S. S., Sulzmann, K. G. P., Ludwig, C. B. (1961): 'Approximate infrared emissivity calculations for NO at elevated temperatures.' *J. Quant. Spectr. Rad. Transfer* **1**, 96–103. [7]

Perrot, F. (1996): 'New approximation for calculating free – free absorption in hot dense plasmas.' *Laser Particle Beams* **14**, 731–748. [13]

Perry, T. S., Davidson, S. J., Serduke, F. J. D., Bach, D. R., Smith, C. C., Foster, J. M., Doyas, R. J., Ward, R. A., Iglesias, C. A., Rogers, F. J., Abdallah Jr., J., Stewart, R. E., Kilkenny, J. D., Lee, R. W. (1991): 'Opacity measurements in a hot dense medium.' *Phys. Rev. Lett.* **67**, 3784–3787. [13]

Perry, T. S., Springer, P. T., Fields, D. F., Bach, D. R., Serduke, F. J., Iglesias, C. A., Rogers, F. J., Nash, J. K., Chen, M. H., Wilson, B. G., Goldstein, W. H., Rozsnyai, B., Ward, R. A., Kilkenny, J. D., Doyas, R., da Silva, L. B., Back, C. A., Cauble, R., Davidson, S. J., Foster, J. M., Smith, C. C., Bar-Shalom, A., Lee, R. W. (1996): 'Absorption experiments on x-ray-heated mid-Z constrained samples.' *Phys. Rev. E* **54**, 5617–5631. [13]

Petsalakis, I. D., Theodorakopoulos, G., Nicolaides, C. A., Buenker, R. J., Peyerimhoff, S. D. (1984): 'Nonorthonormal CI for molecular excited states. I. The sudden polarization effect in 90° twisted ethylene.' *J. Chem. Phys.* **81**, 3161–3167. [5]

Petschek, A., Cohen, H. D. (1972): 'Continuous approximate treatment of ionization potential lowering.' *Phys. Rev. A* **5**, 383–389. [4]

Peyerimhoff, S. D. (1984): 'Calculation of molecular spectra.' *Faraday Symp. Chem. Soc*. **19**, 63–77. [5]

Peyerimhoff, S. D., Buenker, R. J. (1974): 'Ab Initio Calculations for Excited States of Molecules.' In *Chemical Spectroscopy and Photochemistry in the Vacuum-Ultraviolet*. Eds. C. Sandorfy, P. J. Ausloos, M. B. Robin; D. Reidel Publ. Co., Dordrecht-Holland, Boston, p. 257–286. [5]

Peyerimhoff, S. D., Buenker R. J. (1981): 'Electronically excited and ionized states of the chlorine molecule.' *Chem. Phys.* **57**, 279–296. [5]

Peytremann, E. (1974): 'Line-blanketing and model stellar atmospheres. I. Statistical method and calculation of a grid of models.' *Astron. Astrophys.* **33**, 203–214. [7]

Pfennig, H., Trefftz, E. (1966): 'Die Druckverbreiterung der diffusen Heliumlinien, Vergleich Zwischen Messung und Theorie im quasistatischen Bereich.' *Z. Naturforsch.* **21a**, 697–718. [7]

Phillips, R. A., Buenker, R. J. (1987): 'Factors involved in the accurate calculation of oscillator strengths: The $A^1B_1 - X^1A_1$ transition of H_2O.' *Chem. Phys. Lett.* **137**, 157–161. [5]

Picart, J., Edmonds, A. R., Tran Minh, N. (1978): 'Extrapolations to high principal quantum numbers of radial integrals in the Coulomb approximation.' *J. Phys.* **B 11**, L651–L654. [5]

Pierrot, A., Soufian, A., Taine, J. (1999): 'Accuracy of narrow-band and global models for radiative transfer in H_2O, CO_2, and H_2O-CO_2 mixtures at high temperatures.' *J. Quant. Spectr. Rad. Transfer* **62**, 523–548. [7]

Pimpale, A., Mande, C. (1971): 'Influence of plasmons on Compton scattering.' *J. Phys. C* **4**, 2593–2597. [5, 6]

Pines, D. (1955): 'Electron interaction in metals.' *Solid State Physics* **1**, 367–450. [5]

Pines, D. (1963): *Elementary Excitations in Solids*. W. A. Benjamin, Inc., New York, Amsterdam. [5]

Pitzer, K. S. (1981): 'Electron structure of molecules with very heavy atoms using effective core potentials.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 403–420. [3]

Placzek, G. (1934): 'Rayleigh-Streuung und Raman-Effekt.' In *Handbuch der Radiologie*, 3. Kap. (Vol. VI). Ed. E. Marx; Akademische Verlagsgesellschaft, Leipzig. [5]

Planck, M. (1924): 'Zur Quantenstatistik des Bohrschen Atommodells.' *Ann. Phys. (Vierte Folge)* **75**, 673–684. [4]

Plass, G. N. (1958): 'Models for spectral band absorption.' *J. Opt. Soc. Am.* **48**, 690–703. [7]

Plass, G. N. (1960): 'Useful representations for measurements of spectral band absorption.' *J. Opt. Soc. Am.* **50**, 868–875. [7]

Plock, R. J. (1957): 'I. Non-Newtonian Viscoelastic Properties of Rod-Like Macromolecules in Solution. II. The Debye–Hückel, Fermi–Thomas Theory of Plasmas and Liquid Metals.' Ph. D. Dissertation, Yale University, New Haven, CT. [4]

Poll, J. D., van Kranendonk, J. (1961): 'Theory of translational absorption in gases.' *Can. J. Phys.* **39**, 189–204 [8]

Pollack, J. B., Toon, O. B., Khare, B. N. (1973): 'Optical properties of some terrestrial rocks and glasses.' *Icarus* **19**, 372–389. [6]

Pollack, J. B., McKay, C. P., Christofferson, B. M. (1985): 'A calculation of the Rosseland mean opacity of dust grains in primordial solar system nebulae.' *Icarus* **64**, 471–492. [6]

Pollack, J. B., Hollenbach, D., Beckwith, S., Simonelli, D. P., Roush, T., Fong, W. (1994): 'Composition and radiative properties of grains in molecular clouds and accretion disks.' *Astrophys. J.* **421**, 615–639. [6]

Pomraning, G. C. (1971): 'High temperature radiative transfer and hydrodynamics,' In *Progress in High Temperature Physics and Chemistry.* Ed. C. A. Rouse; Pergamon Press, Oxford, New York, Toronto, Sydney, Braunschweig, Vol. 4, p. 1–84. [2]

Pople, J. A. (1982): 'Molecular orbital theories and the structural properties of molecules.' *Ber. Bunsenges. Phys. Chem.* **86**, 806–811. [3]

Pople, J. A., Segal, G. A. (1965): 'Approximate self-consistent molecular orbital theory. II. Calculations with complete neglect of differential overlap.' *J. Chem. Phys.* **43**, S136–S151. [3]

Pople, J. A., Segal, G. A. (1966): 'Approximate self-consistent molecular orbital theory. III. CNDO results for AB_2 and AB_3 systems.' *J. Chem. Phys.* **44**, 3289–3296. [3]

Pople, J. A., Beveridge, D. L. (1970): *Approximate Molecular Orbital Theory*. McGraw-Hill Book Co., Inc., New York, St. Louis, San Francisco, Düsseldorf, London, Mexico, Panama, Sydney, Toronto. [3]

Pople, J. A., Santry, D. P., Segal, G. A. (1965): 'Approximate self-consistent molecular orbital theory. I. Invariant procedures.' *J. Chem. Phys.* **43**, S129–135. [3]

Pradhan, A. K. (1987): 'Opacity project: Astrophysical and fusion applications.' *Phys. Scripta* **35**, 840–845. [5]

Pratt, R. H. (1981): 'Electron bremsstrahlung spectrum.' *Comments At. Mol. Phys.* **10**, 121–131. [6]

Pratt, R. H., Tseng, H. K. (1975): 'Tip region of the bremsstrahlung spectrum from incident electrons of kinetic energy 50 keV–1.84 MeV.' *Phys. Rev. A* **11**, 1797–1803. [5]

Pratt, R. H., Ron, A., Tseng, H.K. (1973): 'Atomic photoelectric effect above 10 keV.' *Rev. Mod. Phys.* **45**, 273–325; **45**, 663–664. [3, 5]

Przybylski, A. (1960): 'On the mean absorption coefficient in the computation of model stellar atmospheres of solar type stars.' *Mon. Not. Roy. Astron. Soc.* **120**, 3–21. [2]

Pugh, L. A., Rao, K. N. (1976): 'Intensities from infrared spectra.' In *Molecular Spectroscopy: Modern Research.* Ed. K. N. Rao; Academic Press, New York, San Francisco, London, Vol. 2, p. 165–227. [5]

Pulay, P. (1977): 'Direct use of the gradient for investigating molecular energy surfaces.' In *Modern Theoretical Chemistry.* Ed. H. F. Schaefer, III; Plenum Press, New York, Vol. 4, p. 153–185. [5]

Pulay, P. (1987): 'Analytical derivative methods in quantum chemistry.' *Adv. Chem. Phys.* **69**, 241–286. [5]

Purcell, E. M., Pennypacker, C. R. (1973): 'Scattering and absorption of light by nonspherical dielectric grains.' *Astrophys. J.* **186**, 705–714. [5]

Pyper, N. C. (1981): 'Relativistic calculations for atoms, molecules and ionic solids: Fully ab-initio calculations and the foundations of pseudo-potential and perturbation theory methods.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 437–488. [3]

Pyykkö, P. (1991): 'Basis set expansion Dirac Fock SCF calculations and MBPT refinement – Comment.' In *The Effects of Relativity in Atoms, Molecules and the Solid State*. Eds. S. Wilson, I. P. Grant, and B. L. Gyorffy; Plenum Press, New York, p. 163–164. [3]

Rabalais, J. W. (1977): *Principles of Ultraviolet Photoelectron Spectroscopy.* Wiley, New York. [5]

Racah, G. (1943): 'Theory of complex spectra. III.' *Phys. Rev.* **63**, 367–382. [7]

Rademacher, H., Reiche, F. (1927): 'Die Quantelung des symmetrischen Kreisels nach Schrödingers Undulationsmechanik. II. Intensitätsfragen.' *Z. Phys.* **41**, 453–492. [5]

Raĭzer, Yu. P. (1959): 'Simple method for computing the mean range of radiation in ionized gases at high temperatures.' *Sov. Phys. - JETP* **10**, 769–771. [11]

Rakavy, G., Ron, A. (1967): 'Atomic photoeffect in the range E_γ = 1–2000 keV.' *Phys. Rev.* **159**, 50–56. [5]

Rapoport, L. P., Lisitsin, V. I., Yazykova, S. M. (1977): 'Semi-empirical calculation method for the variation of electronic transition moments in diatomic molecules.' *J. Phys. B* **10**, 3359–3363. [5]

Raseev, G., LeRouzo, H. (1983): 'Electronic ab initio quantum-defect theory. Low-resolution H_2 photoionization spectrum.' *Phys. Rev. A* **27**, 268–284. [5]

Rauk, A., Barriel, J. M. (1977): 'The computation of oscillator strengths and optical rotatory strengths from molecular wavefunctions. The electronic states of H_2O, CO, HCN, H_2O_2, CH_2O and C_2H_4.' *Chem. Phys.* **25**, 409–424. [5]

Reader, J., Corliss, C. H. (1999): 'Line spectra of the elements.' In *Handbook of Chemistry and Physics*, 80th ed., Ed. D. R. Lide; CRC Press, Boca Raton, p. 10-1–10-87. [5]

Rees, A. L. G. (1947): 'The calculation of potential-energy curves from band-spectroscopic data.' *Proc. Phys. Soc. (London)* **59**, 998–1008. [3]

Reiche, F., Rademacher, H. (1926): 'Die Quantelung des symmetrischen Kreisels nach Schrödingers Undulationsmechanik.' *Z. Phys.* **39**, 444–464. [5]

Reid, R. C., Prausnitz, J. M., Poling, B. E. (1987): *The Properties of Gases and Liquids*. McGraw-Hill, 4^{th} ed. [4]

Reimers, J. R. (2001): 'A practical method for the use of curvilinear coordinates in calculations of normal-mode-projected displacements and Duschinsky rotation matrices for large molecules.' *J. Chem. Phys.* **115**, 9103–9109. [3, 5]

Rhodes, P. (1950): 'Fermi–Dirac functions of integral order.' *Proc. Roy. Soc. London* A **204**, 396–405. [9, App. C]

Richard, C., Gordon, I. E., Rothman, L. S., Abel, M., Frommhold, L., Gustafsson, M., Hartmann, J.-M., Hermans, C., Lafferty, W. J., Orton, G. S., Smith, K. M., Tran, H. (2012): 'New section of the HITRAN database: Collision-induced absorption (CIA).' *J. Quant. Spectr. Rad. Transfer* **113**, 1276–1285. [8]

Richards, W. G., Cooper, D. L. (1983): *Ab Initio Molecular Orbital Calculations for Chemists.* 2^{nd} ed. Clarenden Press, Oxford. [3]

Richards, W. G., Walker, T. E. H., Hinkley, R. K. (1971): *A Bibliography of Ab Initio Molecular Wave Functions.* Oxford University Press, London, Glasgow, New York, Toronto, Melbourne, Wellington, Cape Town, Salisbury, Ibadan, Nairobi, Dar es Salaam, Lusaka, Addis Ababa, Bombay, Calcutta, Madras, Karachi, Lahore, Dacca, Kuala Lumpur, Singapore, Hong Kong, Tokyo. [3, 5]

Richards, W. G., Walker, T. E. H., Farnell, L., Scott, P. R. (1974): *Bibliography of Ab Initio Molecular Wave Functions. (Supplement for 1970–1973).* Oxford University Press, London, Glasgow, New York, Toronto, Melbourne, Wellington, Cape Town, Ibadan, Nairobi, Dar es Salaam, Lusaka, Addis Ababa, Delhi, Bombay, Calcutta, Madras, Karachi, Lahore, Dacca, Kuala Lumpur, Singapore, Hong Kong, Tokyo. [3, 5]

Richards, W. G., Scott, P. R., Colbourn, E. A., Marchington, A. F., (1978): *Bibliography of Ab Initio Molecular Wave Functions. (Supplement for 1974–1977).* Oxford University Press, Oxford, London, Glasgow, New York, Toronto, Melbourne, Wellington, Ibadan, Nairobi, Dar es Salaam, Lusaka, Cape Town, Kuala Lumpur, Singapore, Addis Ababa, Jakarta, Hong Kong, Tokyo, Delhi, Bombay, Calcutta, Madras, Karachi. [3, 5]

Richards, W. G., Scott, P R., Sackwild, V., Robins, S. A. (1981): *Bibliography of Ab Initio Molecular Wave Functions. (Supplement for 1978–1980).* Oxford University Press, Oxford, London, Glasgow, New York, Toronto, Delhi, Bombay, Calcutta, Madras, Karachi, Kuala Lumpur, Singapore, Hong Kong, Tokyo, Nairobi, Dar es Salaam, Cape Town, Melbourne, Wellington, Beirut, Berlin, Ibadan, Mexico City. [3, 5]

Rickert, A. (1993): 'Zustand und optische Eigenschaften dichter Plasmen.' Dissertation Technische Universität München, Max-Planck-Institut report MPQ-175. [13]

Rickert, A. (1995): 'Review of the third international opacity workshop and code comparison study.' *J. Quant. Spectr. Rad. Transfer* **54**, 325–332. [1, 13]
Rickert, A., Meyer-ter-Vehn, J. (1993): 'Modeling of high-Z plasmas and opacities for radiation hydrodynamics simulations.' *Nuovo Cim.* **106** A, 1845–1850. [13]
Robert, D., Bonamy, J. (1979): 'Short range force effects in semiclassical molecular line broadening calculations.' *J. Physique* **40**, 923–943. [7]
Robert, D., Giraud, M., Galatry, L. (1969): 'Intermolecular potentials and width of pressure-broadened spectral lines. I. Theoretical formulation.' *J. Chem. Phys.* **51**, 2192–2205. [7]
Roche, M. (1990): 'On the polyatomic Franck–Condon factors.' *Chem. Phys. Let.* **168**, 556–558. [5]
Rogers, F. J. (1971): 'Phase shifts of the static screened Coulomb potential.' *Phys. Rev. A* **4**, 1145–1155. [4]
Rogers, F. J. (1974): 'Statistical mechanics of Coulomb gases of arbitrary charge.' *Phys. Rev. A* **10**, 2441–2456. [4]
Rogers, F. J. (1979): 'Formation of composites in equilibrium plasmas.' *Phys. Rev. A* **19** 375–388. [4]
Rogers, F. J. (1981): 'Analytic electron – ion effective potentials for $Z \leq 55$.' *Phys. Rev. A* **23**, 1008–1014. [3, 4]
Rogers, F. J., Iglesias, C. A. (1992): 'Radiative Atomic Rosseland Mean Opacity Tables.' *Astrophys. J. Suppl. Ser.* **79**, 507–568. [1, 13]
Rogers, F. J., Graboske Jr., H. C., Harwood, D. J. (1970): 'Bound eigenstates of the static screened Coulomb potential.' *Phys. Rev. A* **1**, 1577–1586. [4]
Rogers, F. J., Wilson, B. G., Iglesias, C. A. (1988): 'Parametric potential method for generating atomic data.' *Phys. Rev. A* **38**, 5007–5020. [3, 5]
Rogers, F. J., Iglesias, C. A., Wilson, B. G. (1992): 'Spin-orbit interaction effects on the Rosseland mean opacity.' *Astrophys. J.* **397**, 717–728. [1, 13]
Roney, R. L. (1994a): 'Theory of spectral line shape. I. Formulation and line coupling.' *J. Chem. Phys.* **101**, 1037–1049. [7]
Roney, R. L. (1994b): 'Theory of spectral line shape. II. Collision time theory and the line wing.' *J. Chem. Phys.* **101**, 1050–1060. [7]
Roney, R. L. (1995): 'Theory of spectral line shapes. III. The Fano operator from near to far wing.' *J. Chem. Phys.* **102**, 4757–4771. [7]
Roothaan, C. C. J. (1951): 'New developments in molecular orbital theory.' *Rev. Mod. Phys.* **23**, 69–89. [3]
Roothaan, C. C. J., Bagus, P. S. (1963): 'Atomic self-consistent field calculations by the expansion method.' *Methods Comp. Phys.* **2**, 47–94. [3]
Rose, M. E. (1937): 'Relativistic wave function in the continuous spectrum for the Coulomb field.' *Phys. Rev.* **51**, 484–485. [5]
Rose, M. E. (1955): *Multipole Fields*. John Wiley & Sons, Inc., New York. [5]
Rose, M. E., Biedenharn, L. C. (1954): 'Theory of the Photoelectric Effect.' Oak Ridge National Laboratory report ORNL-1779. [5]
Rose, S. J. (1992): 'Calculations of the radiative opacity of laser-produced plasmas.' *J. Phys. B* **25**, 1667–1681. [13]
Rose, S. J. (1994): 'A review of opacity workshops.' *J. Quant. Spectr. Rad. Transfer* **51**, 317–318. [13]
Rose, S. J. (1995): 'The effect of degeneracy on the scattering contribution to the radiative opacity.' *Astrophys. J. Lett.* **453**, L45–L47. [6]
Rose, S. J. (2001): 'The radiative opacity at the Sun center – a code comparison study.' *J. Quant. Spectr. Rad. Transfer* **71**, 635–638. [13]
Rosen, B. (1970): 'Spectroscopic data relative to diatomic molecules.' In *Tables Internationales de Constantes Selectionnees*, Vol. 17. Pergamon Press, Oxford, New York, Toronto, Sydney, Braunschweig. [3]
Rosenbluth, M. N., Kaufman, A. N. (1958): 'Plasma diffusion in a magnetic field.' *Phys. Rev.* **109**, 1–5. [9]

Rosenkranz, P. W. (1975): 'Shape of the 5 mm oxygen band in the atmosphere.' *IEEE Trans. Antennas Prop.* **23**, 498–506. [7]
Rosenkranz, P. W. (1985): 'Pressure broadening of rotational bands. I. A statistical theory.' *J. Chem. Phys.* **83**, 6139–6144. [7]
Rosenkranz, P. W. (1987): 'Pressure broadening of rotational bands. II. Water vapor from 300 to 1100 cm^{-1}.' *J. Chem. Phys.* **87**, 163–170. [7]
Rosseland, S. (1924): 'Note on the absorption of radiation within a star.' *Mon. Not. Roy. Astron. Soc.* **84**, 525–528. [2]
Rotenberg, M., Bivins, R., Metropolis, N., Wooten Jr., J. K., (1959): *The 3–j and 6–j Symbols*. Technology Press, MIT. [3]
Rothman, (1981): 'AFGL atmospheric absorption line parameters compilation: 1980 version.' *Appl. Opt.* **20**, 791–795. [7]
Rozsnyai, B. F. (1972): 'Relativistic Hartree–Fock–Slater calculations for arbitrary temperature and matter density.' *Phys. Rev. A* **5**, 1137–1149. [13]
Rozsnyai, B. F. (1973): 'Photoexcitation and photoionization of atoms at arbitrary temperature and matter density.' *J. Quant. Spectr. Rad. Transfer* **13**, 1285–1299. [4, 12]
Rozsnyai, B. F. (1979): 'Computation of free – free Gaunt factors and conductive opacities in hot matter.' *J. Quant. Spectr. Rad. Transfer* **22**, 337–343. [5, 9]
Rozsnyai, B. F. (1982): 'An overview of the problems connected with theoretical calculations for hot plasmas.' *J. Quant. Spectr. Rad. Transfer* **27**, 211–217. [12]
Rozsnyai, B. (1997): 'Collisional-radiative average-atom model for hot plasmas.' *Phys. Rev. E* **55**, 7507–7521. [14]
Rozsnyai, B. F. (2001): 'Solar opacities.' *J. Quant. Spectr. Rad. Transfer* **71**, 655–663. [13]
Rudkjøbing, M. (1947): 'On the Atmospheres of B-stars.' *Publ. Kopenhagen Obs.* Nr. 145. [2]
Ruhoff, P. T., Ratner, M. A. (2000): 'Algorithms for computing Franck–Condon overlap integrals.' *Int. J. Quantum Chem.* **77**, 383–392. [5]
Russell, H. N. (1936): 'Tables for intensities of lines in multiplets.' *Astrophys. J.* **83**, 129–139. [5]
Rydberg, R. (1932): 'Graphische Darstellung einiger bandenspektroscopischer Ergebnisse.' *Z. Physik* **73**, 376–385. [3]
Sakai, T. (1942): 'Thomas–Fermi's equation at any temperature.' *Proc. Phys. Math. Soc. Japan* **24**, 254–260. [4]
Salem, S. I., Panossian, S. L., Krause, R. A. (1974): 'Experimental K and L relative x-ray emission rates.' *Atomic Data Nucl. Data Tables* **14**, 91–109. [5]
Salpeter, E. E. (1961): 'Energy and pressure of a zero-temperature plasma.' *Astrophys. J.* **134**, 669–682. [9]
Salpeter, E. E. (1974a): Unpublished data. [4]
Salpeter, E. E. (1974b): 'Dying stars and reborn dust.' *Rev. Mod. Phys.* **46**, 433–436. [4]
Sampson, D. H. (1959): 'The opacity at high temperatures due to Compton scattering.' *Astrophys. J.* **129**, 734–751. [6, 11]
Sampson, D. H. (1961): 'Radiation relaxation times at high temperatures.' *Astrophys. J.* **134**, 482–499. [6]
Samson, J. A. R. S. (1966): 'The measurement of the photoionization cross sections of the atomic gases.' *Adv. At. Mol. Phys.* **2**, 177–261. [5]
Sapirstein, J. (1998): 'Theoretical methods for the relativistic atomic many-body problem.' *Rev. Mod. Phys.* **70**, 55–76. [3, 5]
Saunders, V. R. (1975): 'An introduction to molecular integral evaluation.' In *Computational Techniques in Quantum Chemistry and Molecular Physics*. Eds. G. H. F. Diercksen, B. T. Sutcliffe, and A. Veillard; Reidel Publ. Co., Dordrecht, p. 347–424. [3]
Saunders, V. R. (1983): 'Molecular integrals for Gaussian type function.' In *Methods in Computational Molecular Physics*. Eds. G. H. F. Diercksen and S. Wilson; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster, Vol. **113**, p. 1–36. [3]
Saunders, V. R., Guest, M. F. (1982): 'Applications of the Cray-1 for quantum chemical calculations.' *Comp. Phys. Comm.* **26**, 389–395. [3]

Sauter, F. (1931a): 'Über den atomaren Photoeffekt bei großer Härte der anregenden Strahlung.' *Ann. Physik* **9**, 217–248. [5]
Sauter, F. (1931b): 'Über den atomaren Photoeffekt in der K-Schale nach der relativistischen Wellenmechanik Diracs.' *Ann. Physik* **11**, 454–488. [5]
Sauter, F. (1933): 'Zur unrelativistischen Theorie des kontinuierlichen Röntgenspektrums.' *Ann. Physik* **18**, 486–496. [6]
Schaefer III, H. F. (1984): *Quantum Chemistry: The Development of Ab Initio Methods in Molecular Electronic Structure Theory.* Clarenden Press, Oxford. [3]
Scheuer, P. A. G. (1960): 'The absorption coefficient of a plasma at radio frequencies.' *Mon. Not. Roy. Astron. Soc.* **120**, 231–241. [6]
Schinke, R. (1993): *Photodissociation Dynamics.* Cambridge University Press, Cambridge. [5]
Schinke, R., Huber, J. R. (1995): 'Molecular dynamics in excited electronic states – Time-dependent wavepacket studies.' In *Femtosecond Chemistry*; Vol. 1. Ed. J. Manz, VCH, Mannheim, New York, Basel, Cambridge, Tokyo, p. 299–319. [5]
Schinke, R., Engel, V., Andresen, P., Häusler, D. (1985): 'Photodissociation of single H_2O quantum states in the first absorption band: Complete characterization of OH rotational and Λ-doublet state distributions.' *Phys. Rev. Lett.* **55**, 1180–1183. [5]
Schuerman, D. W. (1980): *Light Scattering by Irregular Shaped Particles*. Plenum Press, New York, London. [5]
Schwarzschild, M. (1946): 'On the helium content of the Sun.' *Astrophys. J.* **104**, 203–207. [11]
Schweber, S. S. (1961): *An Introduction to Relativistic Quantum Field Theory*. Row, Peterson & Co., New York. [5]
Schwendeman, R. H., Laurie, V. W. (1958): *Tables of Line Strengths for Rotational Transitions of Asymmetric Rotor Molecules*. Pergamon Press, London, New York, Paris, Los Angeles. [5]
Scofield, J. H. (1969): 'Radiative decay rates of vacancies in the K and L shells.' *Phys. Rev.* **179**, 9–16. [5]
Scofield, J. H. (1974a): 'Exchange corrections of K x-ray emission rates.' *Phys. Rev. A* **9**, 1041–1049. [5]
Scofield, J. H. (1974b): 'Hartree–Fock values of L x-ray emission rates.' *Phys. Rev. A* **10**, 1507–1510. [5]
Scofield, J. H. (1974c): 'Relativistic Hartree–Slater values for K and L x-ray emission rates.' *Atomic Data Nucl. Data Tables* **14**, 121–137. [5]
Seaton, M. J. (1955): 'Le calcul approximatif des sections efficaces de photoionisation atomique. II. Une relation entre le défaut quantique et la phase de la fonction d'onde à la limite spectrale.' *Compt. Rend.* **240**, 1317–1318. [3]
Seaton, M. J. (1958): 'The quantum defect method.' *Mon. Not. Roy. Astron. Soc.* **118**, 504–518. [3]
Seaton, M. J. (1962): 'The impact parameter method for electron excitation of optically allowed atomic transitions.' *Proc. Phys. Soc. (London)* **79**, 1105–1117. [7]
Seaton, M. J. (1966a): 'Quantum defect theory. I. General formulation.' *Proc. Phys. Soc. (London)* **88**, 801–814. [3]
Seaton, M. J. (1966b): 'Quantum defect theory. II. Illustrative one-channel and two-channel problems.' *Proc. Phys. Soc. (London)* **88**, 815–832. [3]
Seaton, M. J. (1974): 'Computer programs for the calculation of electron - atom collision cross sections. II. A numerical method for solving the coupled integro-differential equations.' *J. Phys. B* **7**, 1817–1840. [3]
Seaton, M. (1995): *The Opacity Project, Volume 1*. Inst. Of Physics Publishing, Bristol, Philadelphia. [1, 3, 4, 12]
Seery, D. J., Britton, D. (1964): 'Continuous absorption spectra of chlorine, bromine, BrCl, Icl, and IBr.' *J. Phys. Chem.* **68** 2263–2266. [6]
Seitz, F. (1940): *The Modern Theory of Solids* McGraw-Hill Book Company, Inc., New York, London. [4]
Serduke, F. J. D., Minguez, E., Davidson, S. J., Iglesias, C. A. (2000): 'WorkOp-IV summary: lessons from iron opacities.' *J. Quant. Spectr. Rad. Transfer* **65**, 527–541. [1, 13]

Shalitin, D., Ron, A., Reiss, Y. (1982): 'Iron plasma: Sensitivity of photoelectric cross sections to different models and general features of the Fermi–Amaldi-modified model.' *J. Quant. Spectr. Rad. Transfer* **27**, 219–226. [4]

Sharp, C. M. (1984): 'The computation of Franck–Condon factors, R-centroids, and associated quantities in the electronic transitions of diatomic molecules.' *Astron. Astrophys. Suppl. Ser*. **55**, 33–50. [4]

Sharp, C. M. (1988): 'The computation of band strengths of diatomic molecules: Vibrational transitions.' *Astron. Astrophys. Suppl. Ser*. **72**, 355–365. [5]

Sharp, C. M., Huebner, W. F. (1990): 'Molecular equilibrium with condensation.' *Astrophys. J. Suppl. Ser.* **72**, 417–431. [4]

Sharp, C. M., Wasserburg, G. J. (1995): 'Molecular equilibria and condensation temperatures in carbon-rich gases.' *Geochim. Cosmochim. Acta* **59**, 1633–1652. [4]

Sharp, T. E., Rosenstock, H. M. (1964): 'Franck–Condon factors for polyatomic molecules.' *J. Chem. Phys.* **41**, 3453–3463. [5]

Shemansky, D. E., Broadfoot, A. L. (1971): 'Excitation of N_2 and N_2^+ systems by electrons – I. Absolute transition probabilities.' *J. Quant. Spectr. Rad. Transfer* **11**, 1385–1400. [5]

Shenstone, A. G., Russell, H. N. (1932): 'Perturbed series in line spectra.' *Phys. Rev.* **39**, 415–434. [3]

Shepard, R. (1987): 'The multiconfiguration self-consistent field method.' *Adv. Chem. Phys.* **69**, 63–200. [3, 5]

Shevelko, V. P. (1997): *Atoms and their Spectroscopic Properties*. Springer-Verlag; Berlin, Heidelberg, New York. [5]

Schiff, L. I. (1955): *Quantum Mechanics*. 2^{nd} ed., McGraw-Hill Book Co., Inc., New York. [5]

Shifrin, K. S. (1951): 'Scattering of Light in a Turbid Medium.' NASA Tech. Translation, TT F-477, National Aeronautics and Space Administration, Washington, DC. [5]

Shirai, T., Funatake, Y., Mori, K., Sugar, J., Wiese, W. L., Nakai, Y. (1990): 'Spectral data and Grotrian diagrams for highly ionized iron, Fe VIII – XXVI.' *J. Phys. Chem. Ref. Data* **19**, 127–275. [5]

Shirai, T., Sugar, J., Wiese, W. L. (1996): 'Spectral data for selected highly ionized atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo.' *J. Phys. Chem. Ref. Data Monograph* **8** Am. Chem. Soc. and Am. Inst. Phys., Washington, DC. [5]

Shore, B. W., Menzel, D. H. (1968): *Principles of Atomic Spectra*. John Wiley & Sons, Inc., New York, London, Sydney. [3, 7]

Simandiras, E. D., Amos, R. D., Handy, N. C. (1987): 'The analytic evaluation of second-order Mølter-Plesset (MP2) dipole moment derivatives.' *Chem. Phys.* **114**, 9–20. [5]

Singer, S. J., Freed, K. F., Band, Y. (1985): 'Photodissociation of diatomic molecules to open shell atoms.' *Adv. Chem. Phys.* **61**, 1–110. [5]

Singh, N., Mohan, M. (2002): 'Photoionization of excited states of neon-like Mg III.' *Pramana J. Phys.* **58**, 639–646. [5]

Skupsky, S. (1980): 'X-ray line shift as a high-density diagnostic for laser-imploded plasmas.' *Phys. Rev. A* **21**, 1316–1326. [4]

Slater, J. C. (1930): 'Atomic shielding constants.' *Phys. Rev.* **36**, 57–64. [3]

Slater, J. C. (1951): 'A simplification of the Hartree–Fock method.' *Phys. Rev.* **81**, 385–390. [3]

Slater, J. C. (1955): 'One-electron energies of atoms, molecules, and solids.' *Phys. Rev.* **98**, 1039–1045. [3]

Slater, J. C. (1960): *Quantum Theory of Atomic Structure*, Vol. I and II. McGraw-Hill Book Co., Inc., New York, Toronto, London. [3, 5, 7, 12]

Slater, J. C. (1963): *Quantum Theory of Molecules and Solids*, Vol. 1: *Electronic Structure of Molecules*. McGraw-Hill Book Co., Inc., New York, London. [3]

Slater, J. C. (1972): 'Statistical exchange-correlation in the self-consistent field.' *Adv. Quantum Chem.* **6**, 1–92. [3]

Slater, J. C. (1979): *The Calculation of Molecular Orbitals.* Wiley, New York. [3]

Slattery, W. L., Doolen, G. D., DeWitt, H. E. (1980): 'Improved equation of state for the classical one-component plasma.' *Phys. Rev. A* **21**, 2087–2095. [9]

Smith, C. C. (1998): 'Configuration broadening of high-Z transition array profiles.' *J. Quant. Spectr. Rad. Transfer* **59**, 109–116. [13]

Smith, E. W. (1981): 'Absorption and dispersion in the O_2 microwave spectrum at atmospheric pressures.' *J. Chem. Phys.* **74**, 6658–6673. [7]

Smith, K. (1971): *The Calculation of Atomic Collision Processes*. John Wiley & Sons, Inc., New York, London, Sydney, Toronto. [3]

Smith, M. W., Wiese, W. L. (1973): 'Atomic transition probabilities for forbidden lines of the iron group elements. (A critical data compilation for selected lines).' *J. Phys. Chem. Ref. Data* **2**, 85–120. [5]

Sneden, C., Johnson, H. R., Krupp, B. M. (1976): 'A statistical method for treating molecular line opacities.' *Astrophys. J.* **204**, 281–289. [1, 7]

Sobel'man, I. I. (1992): *Atomic Spectra and Radiative Transitions*. Springer-Verlag, Berlin, Heidelberg, New York. Springer Series on Atoms and Plasmas: Volume 12. [5]

Sobel'man, I. I., Vainstein, L. A., Yukov, E. A. (1995): *Excitation of Atoms and Broadening of Spectral Lines*. Springer-Verlag; Berlin, Heidelberg. [5]

Solinger, A. B. (1970): 'Electrical and thermal conductivity in a superdense lattice. I. High-temperature conductivity.' *Astrophys. J.* **161**, 553–559. [9]

Sommerfeld, A. (1927): 'Zur Elektronentheorie der Metalle.' *Naturwiss.* **41**, 825–832. [9]

Sommerfeld, A. (1928): 'Zur Elektronentheorie der Metalle auf Grund der Fermischen Statistik.' *Z. Phys.* **47**, 1–32. [9]

Sommerfeld, A. (1931): 'Über die Bewegung und Bremsung der Elektronen.' *Ann. Physik* **11**, 257–330. [6]

Sorbie, K. S., Murrell, J. N. (1976): 'Theoretical study of the $O(^1D) + H_2(^1\Sigma_g^+)$ reactive quenching process.' *Mol. Phys.* **31**, 905–920. [5]

Southworth, S., Truesdale, C. M., Kobrin, P. H., Lindle, D. W., Brewer, W. D., Shirley, D. A. (1982): 'Photoionization cross sections and photoelectron asymmetries of the valence orbitals of NO.' *J. Chem. Phys.* **76**, 143–151. [5]

Southworth, S. H., Parr, A. C., Hardis, J. E., Dehmer, J. L. (1986): 'Channel coupling and shape resonance effects in the photoelectron angular distributions of the $3\sigma_g^{-1}$ and $2\sigma_u^{-1}$ channels of N_2.' *Phys. Rev. A* **33**, 1020–1023. [5]

Spirko, V. (1983): Vibrational anharmonicity and the inversion potential functions of NH_3.' *J. Mol. Spectr.* **101**, 30–47. [3]

Spitzer Jr., L. (1962): *Physics of Fully Ionized Gases*. 2^{nd} ed., Interscience Publ., Inc., New York, London. [9]

Spitzer Jr., L., Härm, R. (1953): 'Transport phenomena in a completely ionized gas.' *Phys. Rev.* **89**, 977–981. [9]

Springer, P. T., Fields, D. J., Wilson, B. G., Nash, J. K., Goldstein, W. H., Iglesias, C. A., Rogers, F. J., Swenson, J. K., Chen, M. H., Bar-Shalom, A., Stewart, R. E. (1992): 'Spectroscopic absorption measurements of an iron plasma.' *Phys. Rev. Lett.* **69**, 3735–3738. [13]

Springer, P. T., Wong, K. L., Iglesias, C. A., Hammer, J. H., Porter, J. L., Toor, A., Goldstein, W. H., Wilson, B. G., Rogers, F. J., Deeney, C., Dearborn, D. S., Bruns, C., Emig, J., Stewart, R. E. (1997): 'Laboratory measurement of opacity for stellar envelopes.' *J. Quant. Spectr. Rad. Transfer* **58**, 927–935. [13]

Staemmler, V., Palma, A. (1985): 'CEPA calculations of potential energy surfaces for open-shell systems. IV. Photodissociation of H_2O in the $\tilde{A}^1B_1$ state. *Chem. Phys.* **93**, 63–69. [5]

Starace, A. F. (1971): 'Length and velocity formulas in approximate oscillator-strength calculations.' *Phys. Rev. A* **3**, 1242–1245. [5]

Starace, A. F. (1973): 'Comment on "Length and velocity formulas in approximate oscillator-strength calculations".' *Phys. Rev. A* **8**, 1141–1142. [5]

Steele, D., Lippincott, E. R., Vanderslice, J. T. (1962): 'Comparative study of empirical internuclear potential functions.' *Rev. Mod. Phys.* **34**, 239–251. [3]

Stein, S. (1961): 'Addition theorems for spherical wave funtions.' *Quart. Appl. Math.* **19**, 15–24. [5]

Stephens, J. A., Dill, D. (1985): 'Shape-resonance effects mediated by channel interaction: Angular distributions of N_2 $2\sigma_u$ photoelectrons.' *Phys. Rev. A* **31**, 1968–1970. [5]

Stephens, T. L., Losse, J. D., Stull, V. R., Klein, A. L. (1978): 'Molecular Band Models for Thermal and Optically Pumped Emissions.' Defense Nuclear Agency report DNA-3964F-28. [7]

Stewart, J. C. (1965): 'Integrated absorptivity of Gaussian clusters of Lorentz lines.' *J. Quant. Spectr. Rad. Transfer* **5**, 489–493. [7]

Stewart, A. L. (1967): 'The quantal calculation of photoionization cross sections.' In *Advances in Atomic and Molecular Physics.* Eds. D. R. Bates and J. Estermann; Academic Press, New York, Vol. 3, p. 1–52. [1]

Stewart, J. C., Pyatt Jr., K. D. (1961): 'Theoretical Study of Optical Properties.' Air Force Special Weapons Center report SWC-TR-61-71, Vol. 1. [4, 6, 7]

Stewart, J. C., Rotenberg, M. (1965): 'Wave functions and transition probabilities in scaled Thomas–Fermi ion potentials.' *Phys. Rev.* **140**, A1508-A1519; **156**, 230–230. [3, 5, 12]

Stewart, J. C., Pyatt Jr., K. D. (1966): 'Lowering of ionization potentials in plasmas.' *Astrophys. J.* **144**, 1203–1211. [4]

Stobbe, M. (1930): 'Zur Quantenmechanik photoelectrischer Prozesse.' *Ann. Physik* **7**, 661–715. [5]

Stogryn, D. E., Stogryn, A. P. (1966): 'Molecular multipole moments.' *Mol. Phys.* **11**, 371–393. [8]

Stone, N. W. B., Read, L. A. A., Anderson, W. (1984): 'Temperature dependent collision-induced absorption in nitrogen.' *Can. J. Phys.* **62**, 338–347. [13]

Storm, E., Israel, H. I. (1967): 'Photon Cross Sections from 0.001 to 100 MeV for Elements 1 through 100.' Los Alamos Scientific Laboratory report LA-3753. [5]

Stothers, R., Simon, N. R. (1970): 'Influence of opacity on the pulsational stability of massive stars with uniform chemical composition.' *Astrophys. J.* **160**, 1019–1029. [11]

Stratton, J. A. (1941): *Electromagnetic Theory*. McGraw-Hill Book Co., Inc., New York. [5]

Stratton, J. A., Morse, P. M., Chu, L. J., Hutner, R. A. (1941): *Elliptic Cylinder and Spheroidal Wave Functions Including Tables of Separation Constants and Coefficients*. John Wiley & Sons, Inc., New York; Chapman & Hall, Limited, London. [5]

Stratton, J. A., Morse, P. M., Chu, L. J., Little, J. D. C., Corbató, F. J. (1956): *Spheroidal Wave Functions Including Tables of Separation Constants and Coefficients*. John Wiley & Sons, Inc., New York; Chapman & Hall, Limited, London. [5]

Strömgren, B. (1932): 'Opacity of stellar matter and the hydrogen content of stars.' *Z. Astrophys.* **4**, 118–152. [4]

Strom, S. E., Kurucz, R. L. (1966): 'A statistical procedure for computing line-blanketed model stellar atmospheres with applications to the *F* 5 IV star Procyon.' *J. Quant. Spectr. Rad. Transfer* **6**, 591–607. [1, 7]

Strow, L. L., Tobin, D. C., McMillan, W. W., Hannon, S. E., Smith, W. L., Revercomb, H. E., Knuteson, R. O. (1998): 'Impact of a new water vapor continuum and line shape model on observed high resolution infrared radiances.' *J. Quant. Spectr. Rad. Transfer* **59**, 303–317. [7]

Stull, V. R., Plass, G. N. (1960): 'Spectral emissivity of HCl from 1000–3400 cm^{-1}.' *J. Opt. Soc. Am.* **50**, 1279–1285. [7]

Stull, D. R., Prophet, H. (1971): Project Directors, *JANAF Thermochemical Tables* (NSRDS-NBS 37). National Bureau of Standards, Washington, DC. [4]

Sugar, J., Corliss, C. (1985): *Atomic Energy Levels of the Iron-Period Elements, Potassium through Nickel.* National Bureau of Standards, Washington, DC. [3, 4]

Sugar, J., Musgrove, A. (1988): 'Energy levels of molybdenum, Mo I through Mo XLII.' *J. Phys. Chem. Ref. Data* **17**, 155–239. [5]

Sulzer, P., Wieland, K. (1952): 'Intensitätsverteilung eines kontinuierlichen Absorptionsspektrums in Abhängigkeit von Temperatur und Wellenzahl.' *Helv. Phys. Acta* **25**, 653–676. [6]

Sutcliffe, B. T. (1992): 'The Born – Oppenheimer approximation.' In *Methods in Computational Molecular Physics* . Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 19–46. [3]

Sutcliffe, B. T. (1997a): 'The nuclear motion problem in molecular physics.' In *Advances in Quantum Chemistry: Recent Advances in Computational Chemsitry*. Eds. P.-O. Lowden, J. R. Sabin, M. C. Zerner, J. Karwowski, M. Karelson; Academic Press, New York, London, p. 66–81. [3]

Sutcliffe, B. T. (1997b): 'Molecular properties in different environments.' In *Problem Solving in Computational Molecular Science: Molecules in Different Environments.* Ed. S. Wilson and G. H. F. Diercksen. Kluwer; Dordrecht, Boston, London, p. 1–36. [3]

Suvernev, A. A., Goodson, D. A. (1997a): 'Dimensional perturbation theory: an efficient method for computing vibration-rotation spectra.' *Chem. Phys. Lett.* **269**, 177–82. [5]

Suvernev, A. A., Goodson, D. A. (1997b): 'Dimensional perturbation theory for vibration-rotation spectra of linear triatomic molecules.' *J. Chem. Phys.* **107**, 4099–4111. [5]

Swanton, D. J., Bacskay, G. B., Hush, N. S. (1986): 'The infrared absorption intensities of the water molecule: A quantum chemical study.' *J. Chem. Phys.* **84**, 5715–5727. [5]

Synge, J. L. (1957): *The Relativistic Gas*. North-Holland Publ. Co., Amsterdam. [6]

Tatum, J. B. (1967): 'The interpretation of intensities in diatomic molecular spectra.' *Astrophys. J. Suppl. Ser.* **14**, 21–55. [4]

Tatum, J. B. (1971): 'Erratum to the interpretation of intensities in diatomic molecular spectra.' *Astrophys. J. Suppl. Ser.* **22**, 388. [4]

Taylor, P. R., Bacskay, G. B., Hush, N. S. (1976): 'The coupled–pair approximation in a basis of independent–pair natural orbitals.' *Chem. Phys. Lett.* **41**, 444–449. [5]

Taylor, R. L., Caledonia, G. (1969): 'Experimental determination of the cross-sections for neutral bremsstrahlung. I. Ne, Ar and Xe.' *J. Quant. Spectr. Rad. Transfer* **9**, 657–679. [6]

Tellinghuisen, J. (1984): 'On the efficiency and accuracy of quantum and classical methods of calculating diatomic spectra.' *J. Chem. Phys.* **80**, 5472–5474. [7]

Tennyson, J. (1987a): 'Fully vibrationally resolved photoionisation of H_2 and D_2.' *J. Phys. B* **20**, L375–L378. [5]

Tennyson, J. (1987b): 'Calculated vibrationally and rotationally resolved photoelectron spectra of H_2.' In *Electron–Molecule Scattering and Photoionization.* Eds. P. G. Burke and J. B. West; Plenum Press, New York, London, p. 247–251. [5]

Theodorakopoulos, G., Petsalakis, D., Nicolaides, A. (1985a): 'The $\tilde{X}^1A_1 \rightarrow \tilde{A}^1B_1$ transition moment of H_2O using state-specific configuration-interaction wave functions.' *J. Chem. Phys.* **82**, 912–916. [5]

Theodorakopoulos, G., Petsalakis, I. D., Nicolaides, C. A., Buenker, R. J. (1985b): 'Configuration interaction study of the oscillator strengths for the $\tilde{B}^1A_1$-$\tilde{X}^1A_1$ and $\tilde{D}^1A_1$-$\tilde{X}^1A_1$ transitions of the water molecule.' *Chem. Phys*. **100**, 331–337. [5]

Thomas, L. H. (1930): 'Slow expansion or contraction of a fluid sphere.' *Mon. Not. Roy. Astron. Soc.* **91**, 122–127. [2]

Thompson, W. B. (1972): 'The self-consistent test-particle approach to relativistic kinetic theory.' In *General Relativity*. Ed. L. O'Raifeartaigh; Clarendon Press, Oxford, p. 243–254. [6]

Thomson, D. B. (1980): 'An opacity test using a Ne-seeded theta pinch.' *Los Alamos Scientific Laboratory report LA-7684-MS* [13]

Thomson, D. B., Jones, L. A., Bailey, A. G., Engleman Jr., R. (1976): 'Characteristics of high-density theta-pinches seeded with selected high-Z elements.' In *Pulsed High Beta Plasmas.* Ed. D. E. Evans. Pergamon Press; Oxford , New York, p. 209–213. [13]

Thouless, D. J. (1972): *The Quantum Mechanics of Many-Body Systems*. 2^{nd} ed., Academic Press, New York, London. [5]

Tobin, D. C., Strow, L. L., Lafferty, W. J., Olson, W. B. (1996): 'Experimental investigation of the self- and N_2-broadened continuum within the ν_2 band of water vapor.' *Appl. Opt.* **35**, 4724–4734. [7]

Toniolo, A., Persico, M. (2001): 'Efficient calculation of Franck–Condon factors and vibronic couplings in polyatomics.' *J. Comp. Chem.* **22**, 968–975. [5]

Toth, R. A., Hunt, R. H., Plyler, E. K. (1969): 'Line intensities in the 3–0 band of CO and dipole moment matrix elements for the CO molecule.' *J. Mol. Spectr.* **32**, 85–96. [5]

Townes, C. H., Schawlow, A. L. (1955): *Microwave Spectroscopy*. McGraw-Hill Book Co., Inc., New York, Toronto, London. [3, 5]

Traving, G. (1960): *Über die Theorie der Druckverbreiterung von Spektrallinien*. Verlag G. Braun, Karlsruhe. [7]

Truesdale, C. M., Southworth, S., Kobrin, P. H., Lindle, D. W., Shirley, D. A. (1983): 'Photoelectron angular distributions of the N_2O outer valence orbitals in the 19–31 eV photon energy range.' *J. Chem. Phys.* **78**, 7117–7123. [5]

Tsao, C. J., Curnutte, B. (1962): 'Line-width of pressure-broadened spectral lines.' *J. Quant. Spectr. Rad. Transfer* **2**, 41–91. [7]

Tseng, H. K., Pratt, R. H. (1970): 'Comments on the calculation of relativistic bremsstrahlung cross sections.' *Phys. Rev. A* **1**, 528–531. [5]

Tseng, H. K., Pratt, R. H. (1971): 'Exact screened calculations of atomic-field bremsstrahlung.' *Phys. Rev. A* **3**, 100–115. [5]

Tsuji, T. (1966a): 'The atmospheric structure of late-type stars. I. Physical properties of cool gaseous mixtures and the effect of molecular line absorption on stellar opacities.' *Pub. Astron. Soc. Japan* **18**, 127–173. [1]

Tsuji, T. (1966b): 'Some problems on the atmospheric structure of late-type stars.' *Proc. Japan Acad. Tokyo* **42**, 258–263. [1]

Tsuji, T. (1971): 'Effect of molecular line absorptions on stellar opacities.' *Publ. Astron. Soc. Japan* **23**, 553–565. [1]

Tuckwell, H. C. (1970): 'On the validity of the Franck–Condon factor approximation for photoionizing transitions of O_2 ($^3\Sigma_g^-$).' *J. Quant. Spectr. Rad. Transfer* **10**, 653–657. [5]

Tuggle, R. S., Iben Jr., I. (1972): 'On the location of pulsational blue edges and estimates on the luminosity and helium content of RR Lyrae stars.' *Astrophys. J.* **178**, 455–465. [11]

Tully, J. A., Seaton, M. J., Berrington, K. A. (1990): 'Atomic data for opacity calculations: XIV. The beryllium sequence.' *J. Phys. B* **23**, 3811–3837. [3]

Tully, J. C., Berry, R. S., Dalton, B. J. (1968): 'Angular distribution of molecular photoelectrons.' *Phys. Rev.* **176**, 95–105. [5]

Turner, A. G. (1974): *Methods in Molecular Orbital Theory*. Prentice Hall, Englewood Cliffs, NJ. [3]

Underhill, A. B., Waddell, J. H. (1959): 'Stark Broadening Function for the Hydrogen Lines.' National Bureau of Standards, circular 603. [7]

Unno, W. (1952a): 'On the radiation pressure in a planetary nebula. II.' *Publ. Astron. Soc. Japan* **3**, 158–170. [7]

Unno, W. (1952b): 'Note on the Zanstra redistribution in planetary nebulae.' *Publ. Astron. Soc. Japan* **4**, 100–102. [7]

Unsöld, A. (1968): *Physik der Sternatmosphären*. 2^{nd} ed., Springer-Verlag, Berlin, Heidelberg, New York. [2, 11]

van de Hulst, H. C. (1957): *Light Scattering by Small Particles*. John Wiley & Sons, Inc., New York. [5]

van Dishoeck, E. F. (1988): 'Photodissociation and photoionization processes.' In *Rate Coefficients in Astrochemistry*. Eds. T. J. Millar, D. A. Williams; Kluwer, Dordrecht, p. 49–72. [5]

van Dishoeck, E. F., Dalgarno, A. (1983): 'Photodissociation processes in the OH molecule.' *J. Chem. Phys.* **79**, 873–888. [5]

van Dishoeck, E. F., van der Hart, W. J., van Hemert, M. (1980): 'Ab initio studies of the photodissociation processes in positive hydrocarbon ions. I. The methane ion.' *Chem. Phys.* **50**, 45–62. [5]

van Harrevelt, R., van Hemert, M. C. (2000a): 'Photodissociation of water. I. Electronic structure calculations for the excited states.' *J. Chem. Phys.* **112**, 5777–5786. [5]

van Harrevelt, R., van Hemert, M. C. (2000b): 'Photodissociation of water. II. Wave packet calculations for the photofragmentation of H_2O and D_2O in the B band.' *J. Chem. Phys.* **112**, 5787–5808. [5]

van Harrevelt, R., van Hemert, M. C. (2001a): 'Photodissociation of water in the A band revisited with new potential energy surfaces.' *J. Chem. Phys.* **114**, 4953–4962. [5]

van Harrevelt, R., van Hemert, M. C. (2001b): 'A comparative classical-quantum study of the photodissociation of water in the $\overline{\text{B}}$ band.' *J. Phys. Chem. A* **105**, 11480–11487. [5]

van Horn, H. M. (1969): 'Crystallization of a classical, one-component Coulomb plasma.' *Phys. Lett.* **28 A**, 706–707. [9]

van Horn, H. M. (1971): 'Cooling of White Dwarfs.' In *Proceedings International Astronomical Union Symposium No. 42* Ed. W. J. Luyten; Springer-Verlag, Dordrecht, p. 97–115. [App. C]

van Kranendonk, J. (1968): 'Intercollisional interference effects in pressure-induced infrared spectra.' *Can. J. Phys.* **46**, 1173–1180. [8]

van Regemorter, J. (1962): 'Rates of collisional excitation in stellar atmospheres.' *Astron. J.* **136**, 906–915. [7]

van Vleck, J. H. (1951a): 'The coupling of angular momentum vectors in molecules.' *Rev. Mod. Phys.* **23**, 213–227. [3]

van Vleck, J. H. (1951b): 'Klein's theory and the coupling of angular momenta in molecules.' *Phys. Rev.* **82**, 320–320. [3]

van Vleck, J. H., Weisskopf, V. F. (1945): 'On the shape of collision-broadened lines.' *Rev. Mod. Phys.* **17**, 227–236. [7, 8]

Varanasi, P. (1988a): 'Infrared absorption by water vapor in the atmospheric window.' In *Proc. Soc. Photo-opt. Instr. Eng.* **928**, 213–320. [7]

Varanasi, P. (1988b): 'On the nature of the infrared spectrum of water vapor between 8 and 14 μm.' *J. Quant. Spectr. Rad. Transfer* **40**, 169–175. [7]

Varanasi, P., Penner, S. S. (1967): 'Absolute infrared intensity measurements on the fundamental of NO.' *J. Quant. Spectr. Rad. Transfer* **7**, 279–282. [7]

Varandas, A. J. C. (1988): 'Intermolecular and intramolecular potentials: Topographical aspects, calculation, and functional representation via a double many-body expansion method.' *Adv. Chem. Phys.* **74**, 255–338. [3]

Vasileff, H. D. (1954): 'Thermal ionization of impurities in polar crystals. I. Formal theory.' *Phys. Rev.* **96**, 603–609. [7]

Vedenov, A. A., Larkin, A. I. (1959): 'Equation of state of a plasma.' *Zh. Eksper. Teor. Fiz.* **36**, 1133–1142 (*Sov. Phys. - JETP* **9**, 806–811). [4]

Verner, D. A., Yakovlev, D. G. (1995): 'Analytic fits for partial photoionization cross sections.' *Astron. Astrophys. Suppl.* **109**, 125–133. [5]

Verner, D. A., Yakovlev, D. G., Band, I. M., Trzhaskovskaya, M. B. (1993): 'Subshell photoionization cross sections and ionization energies of atoms and ions from He to Zn.' *atomic data Nucl. Data tables* **55**, 233–280. [5]

Vitense, E. (1951): 'Der Aufbau der Sternatmosphären. IV. Teil. Kontinuierliche Absorption und Streuung als Funktion von Druck und Temperatur.' *Z. Astrophys.* **28**, 81–112. [1, 4]

Von Niessen, W., Diercksen, G. H. F., Cederbaum, L. S. (1977): 'On the accuracy of ionization potentials calculated by Green's functions.' *J. Chem. Phys.* **67**, 4124–4131. [5]

von Ragué Schleyer, P. (1998): *Encyclopedia of Computational Chemistry*. Wiley, Chichester, New York. [5]

Voshchinnikov, N. V., Videen, G. (Eds.) (2007): 'IX Conference on Electromagnetic and Light Scattering by Non-sperical Particles.' *J. Quant. Spectr. Rad. Transfer* **106**, 1–622. [6]

Vosko, S. H., Wilk, L., Nusair, M. (1980): 'Accurate spin-dependent electron liquid correlation energies for local spin density calculations: A critical analysis.' *Can. J. Phys.* **58**, 1200–1211. [4]

Wacker, P. F., Pratto, M. R. (1964): *Microwave Spectral Tables, Line Strength of Asymmetric Rotors*. NBS Monograph 70, Vol. II, U. S. Government Printing Office, Washington, DC. [5]

Wahl, A. C., Bertoncini, P. J., Das, G., Gilbert, T. L. (1967): 'Recent progress beyond the Hartree–Fock method for diatomic molecules: The method of optimized valence configurations.' *Int. J. Quantum Chem. Symp.* **1**, 123–152. [3]

Wait, J. R. (1955): 'Scattering of a plane wave from a circular dielectric cylinder at oblique incidence.' *Can. J. Phys.* bf 33, 189–195. [5]

Wallace, S., Dill, D., Dehmer, J. L. (1979): 'Spectral variation of molecular photoelectron angular distributions: Valence shells of N_2 and CO.' *J. Phys. B* **12**, L417–L420. [5]

Wallace, S., Dill, D., Dehmer, J. L., (1982): 'Shape resonant features in the photoionization spectra of NO.' *J. Chem. Phys.* **76**, 1217–1222. [5]

Waller, I., Hartree, D. R. (1929): 'On the intensity of total scattering of x-rays.' *Proc. Roy. Soc. (London), Ser. A* **124**, 119–142. [5]

Wang, H.-T., Felps, W. S., McGlynn, S. P. (1977): 'Molecular Rydberg states. VII. Water.' *J. Chem. Phys.* **67**, 2614–2628. [5]

Warshel, A., Karplus, M. (1972): 'Vibrational structure of electronic transitions in conjugated molecules.' *Chem. Phys. Lett.* **17**, 7–14. [5]

Watanabe, K., Zelikoff, M. (1953): 'Absorption coefficients of water vapor in the vacuum ultraviolet.' *J. Opt. Soc. Am.* **43**, 753–755. [5]

Watson, J. K. G. (1968): 'Simplification of the molecular vibration-rotation Hamiltonian.' *Mol. Phys.* **15**, 479–490. [3]

Watson, J. K. G. (1970a): 'The vibration-rotation Hamiltonian of linear molecules.' *Mol. Phys.* **19**, 465–487. [5]

Watson, W. D. (1969a): 'The effect of auto-ionization lines on the opacity of stellar interiors.' *Astrophys. J.* **157**, 375–387. [5, 12]

Watson, W. D. (1969b): 'The effect of collective interactions on the electron-scattering opacity of stellar interiors.' *Astrophys. J.* **158**, 303–313. [6]

Watson, W. D. (1970b): 'The influence of ion correlations on the free-free opacity of stellar interiors.' *Astrophys. J.* **159**, 653–658. [6]

Weber, J., Hohlneicher, G. (2003): 'Franck–Condon factors for polyatomic molecules.' *Mol. Phys.* **101**, 2125–2144. [5]

Weber, D., Penner, S. S. (1953): 'Rotational line-width measurements on NO, HCl, and HBr.' *J. Chem. Phys.* **21**, 1503–1506. [7]

Weisbach, M. F., Chakerian Jr., C. (1973): 'Line-widths and transition probabilities for the carbon monoxide laser lines.' *J. Chem. Phys.* **59**, 4272–4276. [5]

Weisskopf, V. (1932): 'Zur Theorie der Kopplungbreite und der Stoßdämpfung.' *Z. Physik* **75**, 287–301. [7]

Weisstein, E. W. (1999): *CRC Concise Encyclopedia of Mathematics*. CRC Press, Boca Raton. [7]

Wentzel, G. (1928): 'Die unperiodischen Vorgänge in der Wellenmechanik.' *Physik. Z.* **29**, 321–337. [5]

Werner, H.-J. (1981): 'MCSCF calculation of the dipole moment function of CO.' *Mol. Phys.* **44**, 111–123. [5]

Werner, H.-J. (1987): 'Matrix-formulated direct multiconfiguration self-consistent field and multiconfiguration reference configuration-interaction methods.' *Adv. Chem. Phys.* **69**, 1–62. [3, 5]

Werner, H.-J., Reinsch, E. A. (1981): 'An iterative configuration interaction method with configurations generated from several contracted reference determinants.' In *Proc. 5th Semin. on Computational Methods in Quantum Chemistry*. Eds. T. H. van Duinen and W. C. Niewpoort; MPI Garching,. p. 206–233. [5]

Werner, H.-J., Rosmus, P. (1985): '*Ab initio* calculations of radiative transition probabilities in diatomic molecules.' In *Comparison of Ab Initio Calculations with Experiment: State of the Art*. Ed. R. Bartlett; D. Reidel, Dordrecht, p. 267–324. [3, 5]

Werner, H.-J., Rosmus, P., Reinsch, E.-A. (1983): 'Molecular properties from MCSCF – SCEP wave functions. I. Accurate dipole moment functions of OH, OH^-, and OH^+.' *J. Chem. Phys.* **79**, 905–916. [5]

Werner, H.-J., Kalcher, J., Reinsch, E.-A. (1984): 'Accurate *ab initio* calculations of radiative transition probabilities between the $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'^3\Sigma_u^-$, and $C^3\Pi_u$ states of N_2.' *J. Chem. Phys.* **81**, 2420–2431. [5]

White, H. E., Eliason, A. Y. (1933): 'Relative intensity tables for spectrum lines.' *Phys. Rev.* **44**, 753–756. [5]

White, M. (1982): 'Photoelectron angular distributions from electron–atom collisions.' *Phys. Rev. A* **26**, 1907–1914. [5]

Whitehead, R. J., Handy, N. C. (1975): 'Variational claculation of vibration–rotation energy levels for triatomic molecules.' *J. Mol. Spectr.* **55**, 356–373. [3]
Wickramasinghe, N. C. (1973): *Light Scattering Functions for Small Particles*. Wiley, New York. [5]
Wiese, W. L. (1992): 'Spectroscopic data for fusion edge plasmas.' In *Atomic Plasma - Matter Interaction*. Fusion Data Supplement (APID Series) **2**, 7–13. [5]
Wiese, W. L., Fuhr, J. R. (1975): 'Atomic transition probabilities for scandium and titanium. (A critical data compilation of allowed lines).' *J. Phys. Chem. Ref. Data* **4**, 263–352. [5]
Wiese, W. L., Martin, G. A. (1976): 'Oscillator strength distribution in the lithium isoelectronic sequence.' In *7th Yugoslav Symposium and Summer School on Physics of Ionized Gases*. Inst. of Physics, U. Zagreb, p. 675–700. [5]
Wiese, W. L., Martin, G. A. (1986): 'Atomic transition probabilities.' In *CRC Handbook of Chemistry and Physics*. Ed. R. C. Weart, CRC Press, Boca Raton, p. E328–E363. [5]
Wiese, W. L., Smith, M. W., Glennon, B. M. (1966): *Atomic Transition Probabilities, Volume I, Hydrogen through Neon*. National Standard Reference Data Series, NBS 4 (Category 3), U. S. Government Printing Office, Washington, DC. [5]
Wiese, W. L., Kelleher, D. E., Paquette, D. R. (1972): 'Detailed study of the Stark broadening of Balmer lines in a high-density plasma.' *Phys. Rev. A* **6**, 1132–1153. [4, 13]
Wiese, W. L., Fuhr, J. R., Deters, T. M. (1996): 'Atomic transition probabilities of carbon, nitrogen, and oxygen: A critical data compilation.' *J. Phys. Chem. Ref. Data Monograph* **7** Am. Chem. Soc. and Am. Inst. Phys., Woodbury, NY. [5]
Wigner, E. (1938): 'Effects of the electron interaction on the energy levels of electrons in metals.' *Trans. Faraday Soc.* **34**, 678–685. [4]
Wilkinson, P. G. (1961): 'Molecular spectra in the vacuum UV.' *J. Mol. Spectr.* **6**, 1–57. [12]
Wilkinson, P. G, Mulliken, R. S. (1955): 'Far UV absorption spectra of ethylene and ethylene-D4.' *J. Chem. Phys* **23**, 1895–1907. [12]
Williams, A. R. (1974): 'Multiple scattering theory beyond the muffin-tin approximation.' *Int. J. Quantum Chem. Symp.* **8**, 89–108. [3]
Williams, G. R. J., Langhoff, P. W. (1979): 'Photoabsorption in H_2O: Stieltjes-Tchebycheff calculations in the time-dependent Hartree–Fock approximation.' *Chem. Phys. Lett.* **60**, 201–207. [5]
Williams, G. R. J., Langhoff, P. W. (1981): 'Extended-basis-set RPAE calculations of molecular photoionization cross sections: Theoretical studies of V_π–V_σ interaction in molecular nitrogen.' *Chem. Phys. Lett.* **78**, 21–27. [5]
Williamson, A. J. (1996): 'Quantum Monte-Carlo calculations of electronic excitations.' Thesis, Robinson College, Cambridge. http://www.tcm.phy.cam.ac.uk/~ajw29/thesis/thesis.html
Wilson, S. (1983): 'Basis sets.' In *Methods in Computational Molecular Physics*. Eds. G. H. F. Diercksen and S. Wilson; D. Reidel Publ. Co., Dordrecht, Boston, Lancaster, Vol. **113**, p. 71–93. [3]
Wilson, S. (1984): *Electron Correlation in Molecules*. Clarendon Press, Oxford. [3]
Wilson, S. (1986): *Chemistry by Computer: An Overview*. Plenum, New York. [3]
Wilson, S. (1987): 'Basis sets.' *Adv. Chem. Phys.* **67**, 439–500. [3]
Wilson, S. (1992a): 'The perturbation theory of electron correlation: I. Basic Rayleigh–Schrodinger perturbation theory.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 195–224. [3]
Wilson, S. (1992b): 'The perturbation theory of electron correlation: II. Many-body perturbation theory and the algebraic approximation.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 225–252. [3]
Wilson, S. (1992c): 'The perturbation theory of electron correlation: III. Relativistic many-body perturbation theory.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 253–272. [3]

Wilson, S. (1992d): 'Perturbation theory of electron correlation: IV. Concurrent computation many-body perturbation theory.' In *Methods in Computational Molecular Physics*. Eds. S. Wilson and G. H. F. Diercksen; Plenum Press, New York, London, p. 273–302. [3]

Wilson, S. (1997a): 'Practical ab initio methods for molecular electronic structure studies. I. An overview.' In *Problem Solving in Computational Molecular Science: Molecules in Different Environments.* Ed. S. Wilson and G. H. F. Diercksen. Kluwer; Dordrecht, Boston, London, p. 85–108. [3]

Wilson, S. (1997b): 'Practical ab initio methods for molecular electronic structure studies. II. Finite basis sets and the algebraic approximation.' In *Problem Solving in Computational Molecular Science: Molecules in Different Environments.* Ed. S. Wilson and G. H. F. Diercksen. Kluwer; Dordrecht, Boston, London, p. 109–158. [3]

Wilson, S. (1997c): 'Practical ab initio methods for molecular electronic structure studies. III. Molecular integrals over Gaussian-type functions.' In *Problem Solving in Computational Molecular Science: Molecules in Different Environments.* Ed. S. Wilson and G. H. F. Diercksen. Kluwer; Dordrecht, Boston, London, p. 159–184. [3]

Wilson, S. (1997d): 'Practical ab initio methods for molecular electronic structure studies. IV. Relativistic many-body perturbation theory.' In *Problem Solving in Computational Molecular Science: Molecules in Different Environments.* Ed. S. Wilson and G. H. F. Diercksen. Kluwer; Dordrecht, Boston, London, p. 185–214. [3]

Wilson, S., Silver, D. M. (1976): 'Algebraic approximation in many-body perturbation theory.' *Phys. Rev. A* **14**, 1949–1960. [3]

Wilson, S., Moncrieff, D. (1997): 'Distributed Gaussian basis sets: Some recent results and prospects.' In *Advances in Quantum Chemistry: Recent Advances in Computational Chemistry*. Eds. P.-O. Lowden, J. R. Sabin, M. C. Zerner, J. Karwowski, M. Karelson; Academic Press, New York, London, p. 48–65. [3]

Wilson, S., Diercksen, G. H. F. (Eds.) (1992): *Methods in Computational Molecular Physics*. Plenum Press, New York, London. [3]

Winans, J. G., Stuckelberg, E. C. G. (1928): 'Origin of the continuum spectrum of the hydrogen molecule.' *Proc. Nat. Acad. Sci. USA* **14**, 867–871. [6]

Winhart, G., Eidmann, K., Iglesias, C. A., Bar-Shalom, A., Mínguez, E., Rickert, A., Rose, S. J. (1995): 'XUV opacity measurements and comparison with models.' *J. Quant. Spectr. Rad. Transfer* **54**, 437–446. [13]

Winhart, G., Eidmann, K., Iglesias, C. A., Bar-Shalom, A. (1996): 'Measurements of extreme uv opacities in hot dense Al, Fe, and Ho.' *Phys. Rev. E* **53**, R1332–R1335. [13]

Winstead, C. L. (1987): 'Projection operator formalisms for molecular photoionization resonances using square-integrable basis sets.' Ph. D. Dissertation, Indiana University, Bloomington. [5]

Winstead, C. L., Langhoff, P. W. (1991): 'Feshbach–Fano formalism in Hilbert space: Application to shape resonances in molecular photoionization.' *J. Chem. Phys.* **95**, 3107–3118. [5]

Wiscombe, W., and Mugnai, A. (1980): 'Exact calculations of scattering from moderately-nonspherical T_n-particles.' In *Light Scattering by Irregularly Shaped Particles*. Ed. D. W. Schuerman, Plenum Press, New York, London, p. 141–152. [5]

Wood, M. H. (1974): 'On the calculation of the excited states of small molecules.' *Chem. Phys. Lett*. **28**, 477–481. [5]

Woodall, J., Agúndez, M., Markwick-Kemper, A. J., Millar, T. J. (2007): 'The UMIST database for astrochemistry 2006.' *Astron. Astrophys.* **466**, 1197–1207. [4]

Wyller, A. A. (1962): 'True, ordinary and effective thermal conductivity tensors for a Lorentz-type hydrogen gas.' *Astrophys. Norvegica* **8**, 53–77. [9]

Wyller, A. A. (1973): 'Thermal conductivity of partially degenerate magnetoplasmas in stellar cores.' *Astrophys. J.* **184**, 517–538. [9]

Xu, Y. (1995): 'Electromagnetic scattering by an aggregate of spheres.' *Appl. Optics* **34**, 4573–4588. [5]

Xu, Y. (1996a) 'Fast evaluation of the Gaunt coefficients.' *Math. Comp.* **65**, 1601–1612. [5]

Xu, Y. (1996b) 'Calculation of the addition coefficients in electromagnetic multisphere scattering theory.' *J. Comp. Phys.* **127**, 285–298. [5]

Xu, Y., Gustafson, B. Å. S. (1996): 'A complete and efficient multisphere scattering theory for modeling the optical properties of interplanetary dust.' In *Physics, Chemistry, and Dynamics of Interplanetary Dust*, Eds. B. Å. S. Gustafson, and M. S. Hanner; Astron. Soc. Pacific, Conf. Ser. **104**, p. 419–422. [5]

Yakovlev, D. G. (1984): 'Transport properties of the degenerate electron gas of neutron stars along the quantizing magnetic field.' *Astrophys. Space Sci.* **98**, 37–59. [9]

Yakovlev, D. G. (1987): 'Thermal and electrical conductivities of a degenerate electron gas with electron scattering on heavy ions in the liquid or gaseous phases.' *Astron. Zh.* **64**, 661–664 (Russian). *Sov. Astron.* **31**, 347–348 (English). [9]

Yakovlev, D. G., Urpin, V. A. (1980): 'Thermal and electrical conductivity in white dwarfs and neutron stars.' *Astron. Zh.* **57**, 526–536 (Russian). *Sov. Astron.* **24**, 303–310 (English). [9]

Yamaguchi, Y., Frisch, M., Gaw, J., Schaefer III, H. F. (1986): 'Analytical evaluation and basis set dependence of intensities of infrared spectra.' *J. Chem. Phys.* **84**, 2262–2278. [5]

Yang, C. Y. (1981): 'Relativistic scattered-wave calculations for molecules and clusters in solids.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 335–362. [3]

Yarkony, D. R. (1996): 'Molecular structure.' In *Atomic, Molecular, and Optical Physics Handbook*. Ed. G. W. F. Drake; AIP Press, Woodbury, NY, p. 357–377. [3]

Yeager, D. L. McKoy, V. (1977): 'Transition moments between excited electronic states of N_2^*.' *J. Chem. Phys*. **67**, 2473–2477. [5]

Yeager, D., McKoy, V., Segal, G. A. (1974): 'Assignments in the electronic spectrum of water.' *J. Chem. Phys.* **61**, 755–758. [5]

Yeh, C., Mei, K. K. (1980): 'On the scattering from arbitrarily shaped inhomogeneous particles – Exact solution.' In *Light Scattering by Irregularly Shaped Particles*. Ed. D. W. Schuerman, Plenum Press, New York, London, p. 201–206. [5]

Young, C. (1965): 'Calculation of the absorption coefficient for lines with combined Doppler and Lorentz broadening.' *J. Quant. Spectr. Rad. Transfer* **5**, 549–552. [7]

Young, L. A., Eachus, W. J. (1966): 'Dipole moment function and vibration–rotation matrix elements for CO.' *J. Chem. Phys.* **44**, 4195–4206. [5]

Young, S. J. (1977): 'Nonisothermal band model theory.' *J. Quant. Spectr. Rad. Transfer* **18**, 1–28. [7]

Younger, S. M., Fuhr, J. R., Martin, G. A., Wiese, W. L. (1978): 'Atomic transition probabilities for vanadium, chromium, and manganese. (A critical data compilation of allowed lines).' *J. Phys. Chem. Ref. Data* **7**, 495–629. [5]

Zakrzewski, G., Dolgounitcheva, O., Ortiz, J. V. (1996): 'Direct algorithm for the random-phase approximation.' *Int. J. Quantum Chem.* **60**, 1241–1247. [5]

Zare, R. N. (1964): 'Calculation of intensity distribution in the vibrational structure of electronic transitions: The $B^3\Pi_{0^+u} - X^1\Sigma_{0^+g}$ resonance series of molecular iodine.' *J. Chem. Phys.* **40**, 1934–1945. [3]

Zare, R. N. (1988): *Angular Momentum* Wiley, New York. [5]

Zehe, M. J., Gordon, S., McBride, B. J. (2002): 'CAP: A computer code for generating tabular thermodynamic functions from NASA Lewis coefficients.' Glenn Res. Center, NASA/TP-2001-210959, Rev. 1, Cleveland, Ohio. [4]

Zel'dovich, Ya. B., Raĭzer, Yu. P. (1966): *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*. Vol. 1, Eds. W. D. Hayes and R. F. Probstein; Academic Press, New York, San Francisco, London. [4, 11]

Zel'dovich, Ya. B., Raĭzer, Yu. P. (1967): *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*. Vol. 2, Eds. W. D. Hayes and R. F. Probstein; Academic Press, New York, London. [4]

Zerner, M. C. (1991): 'Semi-empirical molecular orbital methods.' In *Reviews of Computational Chemistry*. Vol. 2. Eds. K. B. Lipkowitz and D. B. Boyd; VCH Publishing, New York, p. 313–366. [3]

Zerner, M. C. (1997): 'On calculating the electronic spectroscopy of very large molecules.' In *Problem Solving in Computational Molecular Science: Molecules in Different Environments.* Ed. S. Wilson and G. H. F. Diercksen. Kluwer; Dordrecht, Boston, London, p. 249–290. [3]

Zhevakin, S. A., Naumov, A. P. (1963): 'Absorption of cm and mm radio waves by the atmospheric water vapor.' *Izvest. Vysshik Uchebn. Zavedenii Radiofiz.* **6**, 674–694 (Russian); (*Radio Eng. Electr. Phys.* **9**, 1097–1105) (English). [7]

Ziegler, T. (1981): 'Calculation of bonding energies by the Hartree – Fock Slater transition state method, including relativistic effects.' In *Relativistic Effects in Atoms, Molecules, and Solids*. Ed. G. L. Malli; Plenum Press, New York, London, p. 421–436. [3]

Ziman, J. M. (1961): 'A theory of the electrical properties of liquid metals. I: The monovalent metals.' *Phil. Mag.* **6**, 1013–1034. [9]

Zink, J. W. (1968): 'Shell structure and the Thomas–Fermi equation of state.' *Phys. Rev.* **176**, 279–284. [4]

Zink, J. W. (1970): 'Energy of partially ionized matter.' *Astrophys. J.* **162**, 145–151. [4]

Zubarev, D. N. (1974): *Nonequilibrium Statistical Thermodynamics*. Consultants Bureau, Plenum Publishing Co., New York. [5]

Zvereva, N. A. (2001): 'Theoretical description of the photodissociation spectrum of monomer and dimer forms of water.' *Optika Spectrosk.* **91**, 640–644 (Russian); *Optics Spectrosc.* **91** 604–608 (English). [5]

Subject Index

W.F. Huebner and W.D. Barfield, *Opacity*, Astrophysics and Space Science Library 402,
DOI 10.1007/978-1-4614-8797-5, © Springer Science+Business Media New York 2014