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Gaseous Ion Mobility, Diffusion, and Reaction

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Notation and Abbreviations

$\mathbf{a}(\mathbf{r},t)$	Acceleration vector as a function of $\mathbf{r}$ and t, Sect. 4.1
$a_{r,s}^{(2T)}$	2T Matrix elements of $\mathfrak{J}_j$ for one gas in a mixture, Sect. 5.6
$a_j^{(MT)}(\cdots)$	MT Matrix elements of $\mathfrak{J}_j$ for one gas in a mixture, Sect. 5.7
a_0	Atomic unit of distance, the bohr, Sect. 6.3
$\mathbf{A}$	Vector potential in Maxwell's equations, Sect. 6.16
$\overline{\mathbf{A}}$	Vector representation of area, Sect. 1.9
A''	Constant used to extract $\overline{\Omega}^{(1,1)}$ from mobility data, Sect. 2.8.4
aug-cc..	cc.. basis set augmented to include diffuse functions, Sect. 6.11.1
b	Impact parameter of a collision, Sect. 1.11
b_1	Ions in a pulse entering the drift tube, Sect. 2.4
$b_{r,s}^{(2T)}$	2T Matrix elements of $\mathfrak{J}_j$ for one gas or a mixture, Sect. 5.6
$b^{(MT)}(\ldots)$	MT Matrix elements of $\mathfrak{J}_j$ for one gas or a mixture, Sect. 5.7
B	Magnetic field strength, Sect. 2.11
$\mathbf{B}$	Magnetic field vector, Sect. 1.15
$B(km;pqst)$	Basis functions of a 2T treatment of molecules, Sect. 8.7
BMM	Beyond Monchick–Mason approximation, Sect. 8.10
BSSE	Basis set superposition error, Sect. 6.11.3
c	Speed of light in a vacuum, Sect. 6.16
$\overline{c}$	Constant term in various equations
$c_{l,m,r}$	Expansion coefficient for $f(\mathbf{r},\mathbf{v},t)$, Sect. 5.4
c_2, c_4	Correction terms in Eq. (1.9), Sect. 1.8
C_3	Coefficient of r^{-3} in long-range potential, Sect. 8.11
C_4	Coefficient of r^{-4} in long-range potential, Sect. 6.22
$\widehat{C}_4$	Value of C_4 in atomic units, Sect. 6.22
C_6	Coefficient of r^{-6} in long-range potential, Sect. 9.1
C_n	Coefficient of r^{-n} in short-range potential, Sect. 9.1.3
cc..	Family of correlation consistent basis functions, Sect. 6.11.1
cc-p	cc basis set with polarized orbitals

cc-pC..	cc basis set with polarized core orbitals, Sect. 6.11.1
cc-pwC..	cc basis set with polarized, weighted core orbitals, Sect. 6.11.1
CAS	Complete active space, Sect. 6.13
CASSCF	Complete active space SCF method, Sect. 6.13
CBS	Complete basis set, Sect. 6.11.1
CC	Coupled-cluster method, Sect. 6.12.1
CI	Configuration interaction, Sect. 6.12.1
CP	Counterpoise correction, Sect. 6.11.3
d	Rigid sphere diameter, Sect. 1.11
d_L	Dimensionless ratio in $f_{rel}(\mathbf{g})$, Sect. 7.2
d_T	Dimensionless ratio in $f_{rel}(\mathbf{g})$, Sect. 7.2
D	Ion diffusion coefficient (a scalar), Sect. 1.9
$\mathbf{D}$	Ion diffusion tensor, Sect. 1.9
D_L	Ion diffusion coefficient along $\mathbf{E}$ or $\mathbf{B}$, Sect. 1.9
D_H	Hall component of $\mathbf{D}$, Sect. 1.15
D_T	Ion diffusion coefficient perpendicular to $\mathbf{E}$, Sect. 1.9
D_x	Same as D_T, Sect. 6.23
D_z	Same as D_L, Sect. 6.23
$D_\parallel$	Same as D_L, Sect. 1.15
$D_\perp$	Same as D_T, Sect. 1.15
d-aug-cc..	cc.. basis set doubly augmented with diffuse functions, Sect. 6.11.1
D	Doubles in a CI calculation, Sect. 6.10
DMS	Differential IMS, Sect. 2.8.4
DTMS	Drift-tube mass spectrometer, Sect. 2.2
e	Fundamental charge, Sect. 2.8.2
E	Electric field strength, Sect. 1.1
$\overline{E}$	Average excess energy in a ping-pong experiment, Sect. 2.9.1
$\tilde{E}$	Time-independent total energy, Sect. 6.3
$\mathbf{E}$	Electric field vector, Sect. 1.8
E_h	Atomic unit of energy, the hartree, Sect. 6.3
E_ion	Ion kinetic energy in swarm frame, Sect. 4.5
E_k	Ion kinetic energy in laboratory frame, Sect. 4.5
E_n	Energy of nth state in perturbation theory, Sect. 6.18
E_p	Electrical potential energy, Sect. 1.3
E_tot	Total energy, Sect. 6.3
$E^{(0)}$	Energy for a simpler problem in perturbation theory, Sect. 6.18
$\widehat{\mathbf{E}}\widehat{\mathbf{E}}$	Energy dyadic in laboratory frame, Sect. 4.5
E/n_0	Reduced field strength, Sect. 1.1
ECP	Effective core potential, Sect. 6.4.6
f	Ion distribution function of many variables, Sect. 8.1
f_c	Fraction of collisions that cool an ion, Sect. 3.5.2
f_h	Fraction of collisions that heat an ion, Sect. 3.5.2
$f(v)$	Ion speed distribution function, Sect. 1.8

$f(\mathbf{v})$	Ion velocity distribution function, Sect. 5.1
$f(\mathbf{r}, \mathbf{v}, t)$	Ion distribution as a function of $\mathbf{r}$, $\mathbf{v}$ and t, Sect. 4.1
$f^{(2T)}(km; .)$	Expansion coefficient for f of molecular ions, Sect. 8.7
$f_0(\mathbf{v})$	Zero-order ion velocity distribution function, Sect. 5.4
$f_0^{(1T)}(\mathbf{v})$	Zero-order ion vdf in 1T theory, Sect. 5.5
$f_0^{(2T)}(\mathbf{v})$	Zero-order ion vdf in 2T theory, Sect. 5.6
$f_0^{(MT)}(\mathbf{v})$	Zero-order ion vdf in MT theory, Sect. 5.7
$f_{GC}(\mathbf{v})$	Gram–Charlier ion vdf, Sect. 7.2
$f_j(\mathbf{v}_j)$	Velocity distribution function of neutral j, Sect. 5.2
$f_R(\mathbf{v}_R)$	Velocity distribution function of reactive neutral R, Sect. 7.1
$f_j(\mathbf{r}, \mathbf{v}_j, t)$	Distribution as a function of $\mathbf{r}$, $\mathbf{v}_j$ and t of neutral j, Sect. 4.2
$f_{rel}(\mathbf{g})$	Relative vdf for an ion–reactive neutral pair, Sect. 7.2
$f_R^{(\beta_R)}(\mathbf{v}_R)$	Vdf of reactive R in state β_R as a function of $\mathbf{v}_R$, Sect. 3.4.3
$f_R(\mathbf{r}, \mathbf{v}_R, t)$	Distribution of reactive R as a function of $\mathbf{r}$, $\mathbf{v}_R$ and t, Sect. 4.3
F	Electrical force, Sect. 1.3
$\mathfrak{F}$	Functional operator, Sect. 5.2
$F(\mathbf{r}, t)$	External force as a function of $\mathbf{r}$ and t, Sect. 4.1
$F_{\|}$	Full width at half height, Sect. 2.4
FAIMS	Field-asymmetric ion mobility spectrometer, Sect. 2.9
g	Relative speed before collision, Sect. 3.2
g'	Relative speed after collision, Sect. 3.3
$\mathbf{g}$	Relative velocity before collision, Sect. 3.3
$\mathbf{g}'$	Relative velocity after collision, Sect. 3.4
$\mathbf{G}$	Center-of-mass velocity before collision, Sect. 3.3
$\mathbf{G}'$	Center-of-mass velocity after collision, Sect. 3.3
GC	Gram–Charlier, Sect. 5.9
GER	Generalized Einstein Relation, Sect. 1.19
h	Planck's constant, Sect. 6.3
H	Hamiltonian operator, Sect. 6.3
H'	Difference operator in perturbation theory, Sect. 6.18
$H^{(0)}$	H for a simpler problem in perturbation theory, Sect. 6.18
H_{int}	Internal Hamiltonian for molecules, Sect. 8.1
$H_p(x)$	Hermite polynomial of order p for variable x, Sect. 5.7
HF	Hartree–Fock method, Sect. 6.8
HPCCS	High Performance Collision Cross Section, Sect. 9.7
i	Base of the imaginary numbers, $\sqrt{-1}$, Sect. 6.3
I	Electric current (in Ch. 1 only), Sect. 1.4
I	Moment of inertia of a molecular ion, Sect. 8.7
I_j	Moment of inertia of a molecule of type j, Sect. 8.5
ICR	Ion cyclotron resonance, Sect. 2.12
IMS	Ion mobility spectrometer, Sect. 2.7
IMS/MS	IMS with a mass spectrometer 2.8
IMoS	Computer program for mobility simulation, Sect. 9.7

IOS	Infinite-order sudden approximation, Sect. 8.10
ITSIM	Computer program for ion trap simulation, Sect. 2.13
$\mathbf{j}$	Ion (or current density) flux vector, Sect. 1.9
j	Index labeling non-reactive gases, Sect. 1.8
$\mathbf{J}$	Pre-collision ion angular momentum vector, Sect. 8.5
$\mathbf{J}^{'}$	Post-collision ion angular momentum vector, Sect. 8.5
$\mathbf{J}_j$	Pre-collision angular momentum vector of j, Sect. 8.5
$\mathbf{J}_j^{'}$	Post-collision ion angular momentum vector, Sect. 8.5
$\mathbf{J}_0$	Angular momentum of a pure neutral gas, Sect. 8.8
$\mathbf{J}_R$	Pre-collision angular momentum vector of R, Sect. 8.5
$\mathfrak{J}_j$	Boltzmann collision operator for neutral j, Sect. 4.2
$\mathfrak{J}_R$	Collision operator for reactive neutral R, Sect. 4.3
k	Reaction rate coefficient, Sect. 1.9
$\widetilde{k}$	Parameter in $V(r)$, Sect. 6.15.3
$k(\mathbf{r}, t)$	Reaction rate coefficient as a function of $\mathbf{r}$ and t, Sect. 4.8
k_{B}	Boltzmann's constant, Sect. 1.9
K	Ion mobility (a scalar), Sect. 1.8
$\mathbf{K}$	Ion mobility (a tensor), Sect. 1.15
$K^{'}$	Logarithmic derivative of K, Sect. 1.19
K_{H}	Hall component of $\mathbf{K}$, Sect. 1.15
K_L	Ion mobility along a magnetic field, Sect. 1.15
K_0	Standard ion mobility (a scalar), Sect. 1.8
$K_{0,n}$	Nominal value of K_0, Sect. 2.2.5
K_T	Ion mobility perpendicular to magnetic field, Sect. 1.15
KE_{cm}	Kinetic energy in the center-of-mass frame, Sect. 7.3
L	Length of apparatus, Sect. 1.1
$\mathbf{L}_0$	Relative angular momentum, Sect. 8.8
$L_r^{(l+1/2)}$	Associated Laguerre polynomial, Sect. 5.5
LCAO	Linear combination of atomic orbitals, Sect. 6.7
LDA	Local density approximation, Sect. 6.2
m	Ion mass, Sect. 1.7
$\widehat{m}$	Ion mass fraction, Sect. 2.7.1
m_j	Mass of neutral j in a mixture, Sect. 5.2
m_0	Neutral mass, Sect. 2.6.1
m_1	Mass of neutral isotope 1, Sect. 2.6.1
m_2	Mass of neutral isotope 2, Sect. 2.6.1
m_R	Mass of reactive neutral R, Sect. 5.2
$\widehat{m}_0$	Neutral mass fraction, Sect. 2.7.1
M	Molar mass of ion, Sect. 1.13
M_R	Molar mass of reactive neutral gas R, Sect. 1.17
M_0	Molar mass of neutral gas molecules, Sect. 1.1
$\overline{M}$	Weighted average of neutral masses, Sect. 2.6.3
MBPT	Many-body perturbation theory, Sect. 6.12.1

MC	Monte Carlo calculation, Sect. 9.4
MCA	Multichannel analyzer, Sect. 2.2.1
MCSCF	Multiconfiguration SCF, Sect. 6.13
MET	Many-electron theory, Sect. 6.20
MMA	Monchick–Mason approximation, Sect. 8.10
MOBCAL	Computer program for mobility calculations, Sect. 9.7
MOBDIF	Computer program for mobility & diffusion, Sect. 6.22.3
MP	Moller–Plesset theory, Sect. 6.19
MP2	Second-order Moller–Plesset theory, Sect. 6.19
MRCI	Multi-reference CI, Sect. 6.14
MS	Mass spectrometer
n	Ion number density, Sect. 1.1
$n(\mathbf{r}, t)$	Ion number density as a function of $\mathbf{r}$ and t, Sect. 4.1
n_j	Number density of gas j in a mixture, Sect. 3.2
n_0	Gas number density, Sect. 1.1
n_R	Number density of reactive gas R, Sect. 4.2
N_G	Normalization factor for Gaussian orbital, Sect. 6.4.1
N_0	Loschmidt's constant, Sect. 1.8
N_S	Normalization factor for Schrodinger orbital, Sect. 6.4.1
$N_{l,m,r}$	Normalization factor for $\Psi_{l,m,r}(\mathbf{v})$, Sect. 5.4
$N_{l,m,r}^{(2T)}$	Normalization factor for $\Psi_{l,m,r}^{(2T)}(\mathbf{v})$, Sect. 5.4
NTE	Nernst–Townsend–Einstein equation, Sect. 1.9
OMEGA	Computer program for collision integrals, Sect. 9.1.3
$\mathbf{p}$	Linear momentum vector, Sect. 6.3
$\overleftrightarrow{\mathbf{p}}$	Four-vector version of $\mathbf{p}$, Sect. 6.17.1
p_j	Component of $\mathbf{p}$ along Cartesian axis j, Sect. 6.3
$P_l^{(m)}$	Associated Legendre polynomial, Sect. 5.5
P_0	Gas pressure, Sect. 1.1
$\widehat{P}_0$	Gas pressure in torr, Sect. 4.7
$P_{0,n}$	Nominal gas pressure, Sect. 2.2.9
PC	Computer program for cross sections, Sect. 5.9
PES	Potential energy surface, Sect. 6.15.1
PUHF	Projected UHF method, Sect. 6.12.3
q	Ion charge, Sect. 1.1
Q	Molar ion charge, Sect. 1.9
$\mathbf{Q}$	Skewness tensor of order three, Sect. 2.4
$\mathbf{Q}_{\mathrm{H}}$	Heat flux vector in laboratory frame, Sect. 4.5
$\mathbf{Q}_{ion}$	Heat flux vector in swarm frame, Sect. 4.5
Q_{RCT}	Cross section of resonant charge transfer, Sect. 6.22.3
Q_R^*	Ion reactive cross section with reactive gas R, Sect. 1.17
$\overline{Q}^{(l)}$	Normalized transport cross section, Sect. 1.11
$\overline{Q}_{\mathrm{eff}}^{(l)}$	Effective $\overline{Q}^{(l)}$ for molecular systems, Sect. 8.11
Qex	Computer program for charge exchange, Sect. 6.22.3

QED	Quantum electrodynamics, Sect. 6.17.1
r	Separation (a scalar), Sect. 1.3
$\mathbf{r}$	Separation vector, Sect. 1.9
$\overleftrightarrow{\mathbf{r}}$	Four-vector version of $\mathbf{r}$, Sect. 6.17.1
$\widetilde{r}$	True minimum of $V(r)$, Sect. 6.15.3
$\mathbf{r}^{(n)}$	Separation vector in space for n electrons, Sect. 6.3
r_A	Separation above which there are no interactions, Sect. 4.2
r_o	Turning point in a collision, Sect. 1.11
r_1	Radius of entrance hole into drift tube, Sect. 2.4
r_2	Radius of exit hole from drift tube, Sect. 2.4
R	Molar gas constant, Sect. 1.9
$\tilde{R}$	Radius of a circular loop, Sect. 6.16
$_R$	Index labeling a reactive neutral, Sect. 1.17
R_t	Resolving power, Sect. 2.5
RASSCF	Restricted active space SCF method, Sect. 6.13
RCC	Restricted coupled-cluster method, Sect. 6.20
RCT	Resonant charge transfer, Sect. 6.22.3
RHF	Restricted Hartree–Fock method, Sect. 6.12.1
S	Total spin quantum number, Sect. 6.12.1
$\mathbf{S}$	Spin angular momentum operator, Sect. 6.6
$S_{l+1/2}^{(r)}$	Sonine polynomial, Sect. 5.5
S	Singles in a CI or CC calculation, Sect. 6.10
SD	S plus doubles, Sect. 6.10
SDT	SD plus triples, Sect. 6.10
SD(T)	SD plus non-perturbative triples, Sect. 6.10
SDTQ	SDT plus quadruples, Sect. 6.10
t	Time, Sect. 1.1
t'	Time needed to reverse an electrostatic field, Sect. 2.9.1
t_d	Time to move from shutter to mass spectrometer, Sect. 2.3.1
$\langle t \rangle$	Average time in drift region, Sect. 1.8
$\langle t \rangle_n$	Nominal average time in drift region, Sect. 2.2.9
T	Ion temperature (a scalar), Sect. 1.13
$\mathbf{T}$	Ion temperature tensor in laboratory frame, Sect. 4.5
T_x, T_y, T_z	Ion temperatures along x, y, and z, Sect. 5.7
T_L	Ion temperature along the field, Sect. 1.19
T_T	Ion temperature perpendicular to the field, Sect. 1.19
$T_{\text{eff},L}$	Effective temperature along the field, Sect. 7.2
$T_{\text{eff},T}$	Effective perpendicular temperature, Sect. 7.2
T_{int}	Internal ion temperature of molecules, Sect. 1.20
$\mathbf{T}_{\text{ion}}$	Ion temperature tensor in swarm frame, Sect. 4.5
T_0	Gas temperature, Sect. 1.1
$\widehat{T}_0$	Gas temperature in kelvin, Sect. 4.7
$T_{0,n}$	Nominal gas temperature, Sect. 2.2.9

T_{eff}	Effective temperature of collisions, Sect. 1.13
T_{kin}	Kinetic ion temperature for molecular ions, Sect. 8.7
T_R	Ion–reactive neutral effective temperature, Sect. 1.17
TM	Trajectory model in MOBCAL, Sect. 9.7
TRAJECK	Computer program for classical trajectories, Sect. 8.9
UHF	Unrestricted Hartree–Fock, Sect. 6.12.3
v	Ion speed (a scalar), Sect. 1.8
$\mathbf{v}$	Ion velocity (a vector), Sect. 1.14
v_{d}	Ion drift speed (a scalar), Sect. 1.8
$\mathbf{v}_{\text{d}}$	Ion drift velocity (a vector), Sect. 1.8
v_i	Ion speed along axis i (a scalar), Sect. 3.2
v_j	Molecular speed of neutral gas j in a mixture, Sect. 4.2
$\mathbf{v}_j$	Velocity vector of neutral gas j in a mixture, Sect. 4.2
v_0	Neutral speed (a scalar), Sect. 3.3
$\mathbf{v}_0$	Neutral velocity vector, Sect. 3.3
$\mathbf{v}_R$	Velocity vector of reactive neutral R, Sect. 7.1
$\mathbf{v}_{R,i}$	Component of $\mathbf{v}_R$ along axis i, Sect. 7.2
$\langle \mathbf{v} \rangle$	Average ion velocity vector, Sect. 1.9
$\langle v \rangle$	Average ion speed before collision, Sect. 3.5.1
$\langle v' \rangle$	Average ion speed after collision, Sect. 3.5.1
$\overline{v}_d$	Average ion drift speed in a ping-pong expt., Sect. 2.9.1
$\overline{\mathbf{v}}_d$	Average ion drift velocity (a vector), Sect. 2.8.1
v_r	Ion speed in the radial direction, Sect. 7.2
v_z	Ion speed along the field, Sect. 3.2
v_{eff}	Effective thermal speed, Sect. 3.4.2
v_{dis}	Displacement of the ion velocity along $\mathbf{E}$, Sect. 5.7
v_{th}	Thermal Speed, Sect. 2.7.1
$V(r)$	Interaction potential energy as a function of r, Sect. 1.11
$V(\mathbf{r})$	V as a function of $\mathbf{r}$, per unit charge, Sect. 6.3
$V(\mathbf{r}, t)$	V as a function of $\mathbf{r}$ and t, per unit charge, Sect. 6.3
V_0	Gas volume, Sect. 1.1
$\widehat{V}_0$	Gas volume bounded by a surface, Sect. 1.9
vdf	velocity distribution function, Sect. 1.14
VDZ	Valence double zeta basis set, Sect. 6.4.2
VXZ	Valence basis set with X = D, T, Q, 5, 6, Sect. 6.4.2
VXZ-PP	A specific version of VXZ, Sect. 6.21
$\mathbf{W}_{1T}$	Dimensionless ion velocity in 1T Theory, Sect. 5.5
$\mathbf{W}_{2T}$	Dimensionless ion velocity in 2T Theory, Sect. 5.6
$\widehat{W}$	Pre-collision ion speed in a special frame, Sect. 3.5.2
$\widehat{W}'$	Post-collision ion speed in a special frame, Sect. 3.5.2
$\widehat{W}_0$	Pre-collision neutral speed in a special frame, Sect. 3.5.2
$\widehat{W}_0'$	Post-collision neutral speed in a special frame, Sect. 3.5.2
WUB	Wang Chang–Uhlenbeck–de Boer equation, Sect. 1.20

x	Integration variable, Sect. 1.11
x_j	Mole fraction of gas j, Sect. 1.8
$Y_l^m(\theta,\phi)$	Spherical harmonic function, Sect. 6.4.1
z	Cartesian axis defined by **E**, Sect. 1.8
z_1	Distance along z, Sect. 2.4
$\widehat{z}$	Dimensionless charge number, Sect. 2.8.2
z_0	Gas compressibility, Sect. 2.2
Z	Partition function of molecular ions, Sect. 1.20
$\widetilde{Z}$	Nuclear charge, Sect. 6.21
Z_0	Partition function of neutral gas molecules, Sect. 3.4.2
Z_R	Partition function of reactive molecules, Sect. 1.20
α	Pre-collision internal state of an ion, Sect. 3.2
α'	Post-collision internal state of an ion, Sect. 8.2
$\boldsymbol{\alpha}$	Vector in Dirac equation, Sect. 6.17.1
$\overleftrightarrow{\boldsymbol{\alpha}}$	Four-vector version of $\boldsymbol{\alpha}$, Sect. 6.17.1
$\widetilde{\alpha}$	Parameter for even-tempered basis set, Sect. 6.4.4
$\alpha(\xi_s)$	First eigenfunction of **S** in spin space, Sect. 6.6
$\widetilde{\alpha}_i$	Determinant coefficients in CI method, Sect. 6.9
$\widehat{\alpha}_0$	Neutral polarizability in cubic Angstroms, Sect. 1.11
α_c	Correction in fundamental ion mobility equation, Sect. 1.11
α_j	Cartesian component of $\boldsymbol{\alpha}$ along axis j, Sect. 6.17.1
α_{T}	Townsend's first ionization coefficient, Sect. 1.10
α_{MT}	Momentum-transfer coefficient, Sect. 3.6
$\alpha_{\parallel}$	Skewness of Gram–Charlier vdf, Sect. 7.2
β	Scalar in Dirac equation, Sect. 6.17.1
$\widetilde{\beta}$	Parameter for even-tempered basis set, Sect. 6.44
β_c	Correction factor in Wannier equation, Sect. 1.13
β_0	Pre-collision internal state of a neutral, Sect. 3.2
β_0'	Post-collision internal state of a neutral, Sect. 8.2
β_R	Pre-collision internal state of a reactive neutral, Sect. 8.2
$\beta(\xi_s)$	Second eigenfunction of **S** in spin space, Sect. 6.6
$\beta_{\parallel}$	Excess kurtosis of the GC vdf along the field, Sect. 7.2
$\beta_{\perp}$	Excess kurtosis perpendicular to the field, Sect. 7.2
$\widetilde{\gamma}$	Parameter for well-tempered basis set, Sect. 6.44
$\boldsymbol{\gamma}$	Dimensionless relative velocity vector, Sect. 3.4.2
γ_i	Component of $\boldsymbol{\gamma}$ along axis i, Sect. 7.2
γ_1	Correlation of speed and energy in GC vdf, Sect. 7.2
γ_2	Correlation of two energies in GC vdf, Sect. 7.2
$\widetilde{\gamma}_1$	First momentum-transfer coefficient, Sect. 3.5.3
$\widetilde{\gamma}_2$	Second momentum-transfer coefficient, Sect. 3.5.3
$\widetilde{\gamma}_3$	Third momentum-transfer coefficient, Sect. 3.5.3
δ_j	Mixture factor for mobility, Sect. 2.5
δ_{P}	Error in gas pressure, Sect. 2.2.9

δ_s	Skewness parameter, Sect. 6.23.5
δ_T	Error in gas temperature, Sect. 2.2.9
δ_ϵ	Error in electromotive force, Sect. 2.2.9
δ_τ	Error in average time in drift region, Sect. 2.2.9
$<\gamma_z(\gamma_z - \gamma_z^{'}) >$	Momentum-transfer collision integral (molecules), Sect. 8.7
$\overline{\epsilon}$	Angle of rotation in a collision, Sect. 4.2
ϵ_{cm}	Center-of-mass collision energy, Sect. 3.3
ϵ_d	Potential well depth, Sect. 9.1.4
ε	Collision energy, Sect. 1.11
ε_V	Electromotive force (emf), Sect. 1.4
$\varepsilon_{V,n}$	Nominal electromotive force, Sect. 2.2.9
ε_0	Electric constant, Sect. 1.3
$\epsilon^{(\alpha)}$	Internal energy of ions in state α, Sect. 1.20
$\epsilon_0^{(\beta)}$	Internal energy of neutrals in state β, Sect. 3.3
ε_R	ϵ_{cm} with reactive neutral R, Sect. 1.17
$\epsilon_R^{(\beta)}$	Internal energy of reactive neutrals in state β, Sect. 1.20
ϵ_{rot}	Pre-collision rotational energy, Sect. 8.8
ζ	Dimensionless orbital exponent (zeta parameter), Sect. 6.4.1
ζ_i	Value of ζ for orbital i, Sect. 6.4.4
ζ_{MT}	Momentum-transfer correlation coefficient, Sect. 3.2
$\zeta(v)$	Druyvesteyn distribution function for electrons, Sect. 1.14
η_l	Phase shift for quantum number l, Sect. 6.22.2
θ	Polar scattering angle of an ion, Sect. 1.11
θ_0	Polar scattering angle of a neutral, Sect. 3.5.3
κ	Correction factor for gas temperature, Sect. 2.2.5
$\widetilde{\kappa}$	Wave number, Sect. 6.22.2
$\widehat{\kappa}$	Anisotropy of ion-dipole potential, Sect. 8.11
μ_j	Reduced mass for ions with a molecule of type j, Sect. 5.8.2
μ_0	Reduced mass for ions with a pure neutral gas, Sect. 1.11
$\widehat{\mu}_0$	Ion–neutral reduced mass in Da (g/mole), Sect. 1.11
μ_R	Reduced mass of ion–reactive neutral system, Sect. 1.17
$\nu^{(1)}$	Microscopic version of $\widetilde{\nu}^{(1)}$, Sect. 2.6.3
$\widetilde{\nu}^{(1)}$	Collision frequency for momentum transfer, Sect. 1.14
ξ	Effective collision frequency, Sect. 2.13
ξ_s	Coordinate for spin space, Sect. 6.6
$\xi^{(1T)}$	Collision frequency for ions in 1T theory, Sect. 5.8
$\xi_j^{(1T)}$	Collision frequency for ions in gas j in 1T theory, Sect. 5.8
$\xi^{(2T)}$	Collision frequency for ions in 2T theory, Sect. 5.8
$\xi_j^{(2T)}$	Collision frequency for ions in gas j in 2T theory, Sect. 5.8
$\xi^{(3T)}$	Collision frequency for ions in 3T theory, Sect. 5.8
$\xi_j^{(3T)}$	Collision frequency for ions in gas j in 3T theory, Sect. 5.8

$\boldsymbol{\pi}$	Kinetic momentum vector, Sect. 6.17.1
ρ	Charge or electron density, Sect. 6.2
σ	Differential scattering cross section, Sect. 1.13
σ_1	Standard deviation of pulse entering drift tube, Sect. 2.4
$\sigma_\parallel$	Standard deviation of arrival times along field, Sect. 2.4
$\sigma^{(\lambda,\upsilon)}$	Cross section of atomic ions in diatoms, Sect. 8.8
τ	Collection of four variables: x, y, z, t, Sect. 6.18
τ_c	Mean time between collisions, Sect. 1.8
ϕ	Azimuthal scattering angle of an ion, Sect. 3.4.1
ϕ_0	Azimuthal scattering angle of a neutral, Sect. 3.5.3
$\phi_{\mathbf{J}}$	Phase angle of $\mathbf{J}$, Sect. 8.8
$\phi_{\mathbf{L}}$	Phase angle of $\mathbf{L}$, Sect. 8.8
φ	Index specifying one nucleus in a molecule, Sect. 6.3
$\boldsymbol{\chi}$	Dimensionless center-of-mass velocity vector, Sect. 3.4.2
ω	Frequency of an ac field, Sect. 2.11
ω_i	Weighting factor in MMA and BMM, Sect. 8.11
ω_j	Weighting factor for average mass, Sect. 2.6.3
Γ	Gamma function, Sect. 1.14
$\Gamma^{(+)}$	Rate of gain of ions in phase space, Sect. 4.1
$\Gamma^{(-)}$	Rate of loss of ions in phase space, Sect. 4.1
Δp_z	Change in ion momentum along the field, Sect. 3.2
Δt	Period of time, Sect. 1.4
$\Delta\varepsilon$	Change in energy, Sect. 1.4
$\Delta\varepsilon_{\text{int}}$	Change in internal energy, Sect. 3.3
Δ_1	Ratio of molecular collision integrals, Sect. 8.7
Δ_L	Correction term in GER for D_L/K, Sect. 1.19
Δ_T	Correction term in GER for D_T/K, Sect. 1.19
Δv_z	Change in ion speed along the field, Sect. 3.2
Υ_{MT}	Momentum-transfer correction factor, Sect. 3.6
Φ	Ratio of collision integrals for molecular systems, Sect. 1.20
$\psi_{n,l,m}$	Slater or Gaussian orbital, Sect. 6.4.1
$\psi^{(0)}$	Wave function for a simpler problem, Sect. 6.18
$\Psi(\mathbf{r},t)$	Position and time-dependent wave function, Sect. 6.3
$\Psi(\mathbf{r})$	Position-independent wave function, Sect. 6.3
$\Psi(\mathbf{r}^{(n)})$	$\Psi(\mathbf{r})$ for n electrons, Sect. 6.3
$\Psi_{l,m,r}(\mathbf{v})$	Generalized basis function of velocity, Sect. 5.4
$\Psi^{(1T)}_{l,m,r}(\mathbf{v})$	$\Psi_{l,m,r}(\mathbf{v})$ in 1T Theory, Sect. 5.5
$\Psi^{(2T)}_{l,m,r}(\mathbf{v})$	$\Psi_{l,m,r}(\mathbf{v})$ in 2T Theory, Sect. 5.6
$\Psi^{(MT)}_{l,m,r}(\mathbf{v})$	$\Psi_{l,m,r}(\mathbf{v})$ in MT Theory, Sect. 5.7
Ω	Molecular momentum-transfer collision integral, Sect. 1.20
$\Omega_d/\widehat{z}$	Structure factor, Sect. 2.8.2
$\overline{\Omega}^{(l,s)}$	Normalized collision integral for atoms, Sect. 1.11

$\overline{\Omega}^{(1,1)}$	Momentum-transfer collision integral for atoms, Sect. 1.11
$\overline{\Omega}^{(l,s)}_{\mathrm{mol}}$	Normalized collision integral for molecules, Sect. 3.4.2
∇	Gradient operator (vector) in space, Sect. 1.9
$\nabla_{\mathbf{v}}$	Gradient operator (vector) in velocity space, Sect. 4.1
∇_x	Component of ∇ along direction x, Sect. 1.9
∇^2	Laplacian operator (scalar), Sect. 1.9
$\mathfrak{N}$	Number of collisions, Sect. 3.5.1
$\odot$	Contraction operator for two tensors, Sect. 1.15
$\overleftrightarrow{\boxdot}$	Four-vector version of ∇ and $\frac{\partial}{\partial t}$, Sect. 6.17.1
$\frac{\partial}{\partial x}$	Partial derivative with respect to any quantity, x, Sect. 1.9
$\cdot$	Scalar product of two vectors (dot product), Sect. 1.9
$\times$	Cross product of two vectors (vector product), Sect. 5.1
$[\ ,\ ]$	Commutator or Poisson bracket, Sect. 8.1
$[p;q]^{(l)}$	Irreducible collision integrals of 3T theory, Sect. 5.7
$[p,q,r\|s,t,u]$	Irreducible collision integrals of MT theory, Sect. 5.8
$\begin{pmatrix} k' \\ k \end{pmatrix}$	Matrix element for diatomic systems, Sect. 8.7

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Crookes	api.ning.com/files/vRWi3e17RGo7u0-6VqhffF1v*Kc AznnHzhH-ltjVJgrpo*l*c6lrrmdHYJDHMgDp3E wsIGdEGK7dB6TMQhEJoVS9-iBP98kQ/Croo.gif
Curtiss	www.chem.wisc.edu/deptfiles/docs/badger-chemist/BChemist_08.pdf
Davy	www.wikigallery.org/paintings/201501-202000/201847/painting1.jpg
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Du Fay	images.fineartamerica.com/images-medium-large/charles-dufay-du-fay1698-1739-sheila-terry.jpg
Einstein	3.bp.blogspot.com/_2BiG4q7GCqk/TTHot-b6_mI/AAAAAAAAB2M/Lq1m4BviklI/s1600/Albert_Einstein_Photo+II.jpg
Enskog	www-history.mcs.st-and.ac.uk/PictDisplay/Enskog.html
Eyring	upload.wikimedia.org/wikipedia/commons/5/54/Henry_B._Eyring2.jpg
Faraday	media.gettyimages.com/photos/portrait-of-michael-faraday-british-chemist-and-physicist-painting-by-picture-id164083627
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Lamb	upload.wikimedia.org/wikipedia/commons/7/77/Willis_Lamb_1955.jpg
Landau	www-history.mcs.st-andrews.ac.uk/BigPictures/Landau_Lev_9.jpeg
Langevin	upload.wikimedia.org/wikipedia/commons/c/cd/Paul_Langevin_Wellcome.jpg
Lenard	upload.wikimedia.org/wikipedia/commons/1/1d/Phillipp_Lenard_in_1900.jpg
Lifshitz	www-history.mcs.st-and.ac.uk/BigPictures/Lifshitz.jpeg
Loeb	en.wikipedia.org/w/index.php?curid=53508692
Loschmidt	www.converter.cz/fyzici/images/loschmidt.jpg
Mack	chemistry.osu.edu/sites/chemistry.osu.edu/files/styles/full_width/public/Edward%20Mack%20Jr.jpg?itok=tTT-dKAH
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Schwinger	upload.wikimedia.org/wikipedia/commons/3/3c/Schwinger.jpg
Sinanoglu	www.itusozluk.com/image/oktay-sinanoglu_17444.jpg
Slater	web.mit.edu/physics/images/history/slater.jpg
Stern	upload.wikimedia.org/wikipedia/commons/6/6e/Otto_Stern_1950s.jpg
Stoney	www.ssplprints.com/image.php?imgref=10309421
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Thomson	www.wired.com/images_blogs/thisdayintech/2012/04/jj_thompson_400px.jpg
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Van de Graaf	tvdg10.phy.bnl.gov/vandegraaff.html
Varley	upload.wikimedia.org/wikipedia/ru/c/c9/Cromwell_Fleetwood_Varley.jpg
Volta	techstory.in/wp-content/uploads/2016/02/Alessandro-Volta.jpg
Waldmann	https://www.mpic.de/uploads/pics/Waldmann_Ludwig_web2.jpg
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Wannier	fr.cdn.v5.futura-sciences.com/builds/images/rte/RTEmagicC_wannier_gregory_AIP_Emilio_Segre_Visual_Archives_Physics_Today_Collection.jpg
Watson	cdn.quotationof.com/images/william-watson-5.jpg
Wiechert	nuclearplanet.com/Final2%20Emil_Wiechert.jpg
Wien	https://upload.wikimedia.org/wikipedia/commons/d/dd/Wilhelm_Wien_1911.jpg
Zeleny	history.aip.org/phn/Photos/zeleny_john_a1.jpg

Preface

This book is about the drift, diffusion, and reaction of ions moving through gases under the influence of an external electric field, the gas temperature, and the number density. Late in the nineteenth century, research in this area helped to establish the existence of electrons and ions and laid the foundation of modern physics and chemistry. Experimental and theoretical studies of ion and electron swarms continue to be important in such varied fields as atomic and molecular physics, aeronomy and atmospheric chemistry, gaseous electronics, plasma processing, and laser physics. In short, there is more that unites all of these research and application areas than the emphases, terminology, and details that separate them. This book is directed toward graduate students and researchers new to this research field, particularly those involved with ion mobility spectrometry and the use of ion transport coefficients to test and improve ab initio ion–neutral interaction potentials.

Surveys of the early history of charged particle transport in gases are given by Loeb (1955), Beynon and Morgan (1978), and others. The early literature is covered so thoroughly by Loeb that in most places in this book the original literature will be cited only if it was published after 1950.

There are three books that may be considered predecessors of the present work, since they are similar in spirit to it. They are by McDaniel and Mason (1973), Huxley and Crompton (1974), and Mason and McDaniel (1988). The titles of these books reflect the unfortunate fact that the transport of electrons and ions has been treated separately for many years. Although there are both theoretical and experimental reasons for this, the two subdisciplines have more in common than is generally appreciated. Accordingly, this book was originally going to treat electrons and ions on an equal basis, similar to the approach used by Kumar et al. (1980), Robson (2006), and Konovalov et al. (2017) in works that can be considered as introductions to the present book. However, this work quickly grew beyond acceptable limits. In addition, a recent book by Robson et al. (2018) treats the transport of any type of charged particle in both gases and condensed matter, albeit

with less detail and from a more advanced starting point than we propose to use here. Therefore, we reluctantly had to limit the majority of this book to swarms of atomic and molecular ions.

Chapter 1 of the book expands upon an encyclopedia article (Viehland 2003) to give a history of swarm research, including information about electron swarms. At the same time, it introduces the basic concepts, physical relationships, and mathematical equations that will be used in the remaining sections. This history emphasizes swarm research connected to physical chemistry and chemical physics. The history of swarm research of interest to analytical chemists is covered by Eiceman et al. (2014).

Chapter 2 discusses the experimental techniques used to study gaseous ion transport, paying more attention to the techniques presently being used than to the older techniques discussed at length in the books mentioned above and focusing more on the theoretical implications of the equipment used. Here too, it was necessary to limit the focus, not only because of space limitations but also because the author's expertise is more in the realm of theory.

Chapter 3 presents momentum-transfer theory, an elementary theory of ion mobility. This introduces the reader to the thinking that undergirds the kinetic theory of swarms and makes clear some of the limitations of the fundamental low-field ion mobility equation.

The kinetic theory of gases is the subset of statistical mechanics that uses the Boltzmann kinetic equation to describe the nonequilibrium properties of a dilute gas. Chapter 4 discusses the Boltzmann equation for atomic ions in atomic gases, thus deferring treatment of molecular ions and neutrals until later in the book.

Solving the Boltzmann equation exactly can be done only for models of the ion motion in gases, not for the general cases of interest here. We begin the process of successive approximations to its solution in Chap. 5, by discussing moment theories. These methods are based on Maxwell's equations of change that are equivalent to Boltzmann's equation. This chapter includes a discussion of what is now considered the standard approach to gaseous ion mobility and diffusion, here called the two-temperature (2T) theory.

The big problem with the 2T theory is that it cannot handle situations that are inherently anisotropic. This problem led to the development of the three-temperature (3T) and Gram–Charlier (GC) theories that are described in Chap. 5. Both use three temperatures: the gas temperature, an ion temperature characterizing the average kinetic energy along the direction of the electrostatic field, and a different ion temperature characterizing the average energy perpendicular to the field. They allow the ion mobility and diffusion coefficients to be calculated from an ion–neutral interaction potential in a series of successive approximations.

Chapter 6 discusses how ion–neutral interaction potentials for atomic ion–atom systems can be calculated ab initio, and how from such potentials the transport coefficients can be calculated ab initio using GC theory. These calculations proceed in a systematic series of approximations starting from a guess for the ion velocity

distribution function (vdf). This guess (called a zero-order approximation of the vdf) involves not only the ion velocity and temperatures but also quantities that in statistics are called skewness and kurtosis. In addition, it allows for correlation between ion properties parallel and perpendicular to the field.

Chapter 7 first discusses the application of the 2T theory to the analysis and understanding of gaseous ion–neutral reaction. It then considers how the vdf for atomic ions moving through atomic gases can be visualized from GC theory and used to compute rate coefficients for chemical reactions of the ions with small amounts of a reactive molecular gas that are included with the neutral buffer gas. It ends by showing that in some cases the reaction cross sections inferred in the past from swarm studies are in error by more than 30%.

Chapter 8 is devoted to changes that occur when either the ion or neutral is molecular. It moves then to a discussion of various extensions of the Boltzmann equation that have been proposed. Only the fully classical extension is presently useful for swarm studies, because the matrix elements of the collision operators used in the other extensions are too difficult to compute. Ab initio calculations are then described for atomic ions in diatomic neutrals and for diatomic ions in atomic neutrals. While such calculations are feasible, they are still so difficult that alternative methods are desirable. The chapter ends with a discussion of the MMA approximation (Monchick and Mason 1961) and the extension of it (Viehland and Chang 2012) that is known as the BMM, for beyond Monchick–Mason. Although still in its infancy, the BMM shows promise of being simple (hence using small amounts of computer power) and accurate enough to test interaction potential energy surfaces.

Chapter 9 starts by describing atomic models that have been used to describe molecular systems. All such models have significant weakness, so this chapter also describes Monte Carlo and molecular dynamics calculations for molecular systems. The final chapter contains a short summary of this book, along with a prediction for the things that lie ahead in a research area that already is more than 120 years old.

It is essential in this book to use a fair amount of mathematics. When calculus is used, the derivations are done slowly so that readers whose calculus skills have weakened with time can have their memories refreshed. In this regard, Appendix A is particularly important, as it explains the mathematical terminology, particularly the terminology of vector calculus, that is crucial to the understanding of swarm experiments but may be unfamiliar to some readers. Appendix B discusses atomic term symbols that are used throughout this book to specify a particular state of an atomic ion or neutral. Unless specifically indicated otherwise, the neutral gases are assumed to be the naturally occurring mixture of the various isotopes. Appendix C discusses the method of weighted residuals that can be used to solve the time-independent Schrödinger equation, the Boltzmann equation, or indeed any mathematical equation involving a linear operator.

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