

Index

A

Ab initio calculations, 129, 139
Asymptotic approximation, 91
ATP, 45
 synthase, 45

B

Basis set superposition error, 24, 49, 218
Boltzmann statistics, 20
Boson, 19, 20

C

Cell model, 104, 159
Chirality, 45
Cluster, 20–26, 121–123
 hydrogen fluoride, 129–133
 population, 22, 23, 25–30, 123, 157, 158, 200
 water, 123–129, 137, 200
Configurational integral, 7, 108, 123
Cooperativity, 126, 132, 148, 185, 189, 190, 199, 201
Cratic correction, 106, 107, 110

D

Decomposition
 entropy, 64, 65, 69, 70, 77–79, 203–206
 Hamilton operator, 12
Degeneracy, 19

E

Ensemble
 canonical, 26, 32

Ensemble average, 34, 36, 38
Enthalpy, 54, 58, 62, 181–183
 association, 57–59, 61
 vibrational, 54, 56, 59, 60
Enthalpy–entropy compensation, 78
Entropy, 30, 54, 58, 61, 62, 66–69, 154, 161, 162
 association, 54, 58, 60, 66–68, 73, 108, 109, 113
 cluster, 156
 electronic, 67
 mixing, 107
 Molar, 156, 159, 161–169, 178, 195–198, 205
 QCE, 31, 32
 rotational, 54–57, 59, 60, 66, 67, 69, 70, 73–77, 96, 98
 solvation, 79, 80
 translational, 54–57, 59, 60, 66, 67, 69, 70, 73–77, 87–97, 105–107, 111, 112, 205
 vaporization, 179, 180, 194, 195, 198–200
 vibrational, 54–57, 59, 60, 66, 67, 69–71, 82, 83, 98–100
Equipartition theorem, 15, 55, 56, 84
Error function, 88, 95–100
Error vector, 25
Excluded volume
 parameter, 123, 152, 153

F

Fermion, 19, 20
Fluctuations, 22, 38
Free energy, 26, 27, 32, 54, 56, 61
Free energy perturbation, 33, 38

G

Gaussian-type integral, 6, 14
Group contribution
 methods, 2

H

Hamilton function, 6, 17
Hamilton operator, 7, 8, 12, 13,
 18, 105
Harmonic approximation, 18, 22, 82, 92
Harmonic oscillator, 17, 70, 82,
 100, 109
Heat capacity, 32, 38, 181, 184, 198
High temperature limit, 14, 15, 19, 20,
 84, 86, 91
Hindered rotor, 102, 104
Hydrogen bond number, 122

I

Ideal gas, 2, 3, 6, 28, 69, 83, 96, 106, 135,
 136, 141, 158, 171
Indistinguishability, 4, 69, 203, 204
Interaction energy, 24, 25, 52, 134
 hydrogen fluoride cluster, 131
 pair, 124, 125, 128
 pseudorotaxanes, 48, 49, 51, 52
 water cluster, 124

J

Jarzynski equality, 39

K

Kinetic energy, 15

L

Localization, 133

M

Mean field parameter, 23, 147
Mechanical bond, 43, 44
Microsolvation, 52, 62, 78, 98, 102
Microstate, 19
Molecular dynamics
 simulations, 32, 33
Molecular machine, 44
Molecular motor, 44
Multinomial theorem, 10
Multiscale approach, 2

N

Normal mode analysis, 18, 79, 93, 94, 100,
 109, 144
Number density, 25, 74, 75, 94, 96, 111

O

Occupation number, 9, 10
Order parameter, 35, 36, 38, 39

P

Parameter adjustment, 189
Particle in a box, 22, 68, 86
Particle number effect, 64, 65, 76
Partition function, 20, 21, 26–28, 30, 32, 33,
 37, 52, 68–70, 81–84, 88, 89, 91,
 102, 103, 185, 203, 204
 electronic, 19, 93, 103, 158
 QCE, 30, 32, 204, 205
 rotational, 15–17, 19, 55, 60, 83, 91
 RRHO model, 68, 69, 83
 translational, 14–16, 24, 69, 81, 83–87, 91,
 96, 158
 vibrational, 17, 18, 92, 93, 185
Peacemaker program, 28–30
Phase space, 34, 35
Population polynomial, 29
Potential
 chemical, 26, 31
 interaction, 8, 33, 77, 103, 108
 mean field, 23, 24, 103, 141, 142, 144, 145,
 147, 152, 153, 161, 162
Probability distribution, 34, 35, 40
Pseudorotaxane, 44–55, 57, 58, 60–63, 66–68,
 110–113, 116

Q

QCE model, 5, 122

R

Rigid rotor, 15–17, 22, 92, 102
RRHO model, 5, 43, 54, 64, 65, 68, 78, 79, 81,
 82, 104, 107, 110

S

Sackur–Tetrode equation, 69, 88
Schrödinger equation, 1, 7–9, 12, 18, 19, 105
Second law of thermodynamics, 39
Shared electron number, 49, 218
Shuttling, 44

Statistical mechanics, 1
Stirling's approximation, 26, 31, 69,
88, 91, 92
Stopper, 44
Symmetry number, 16, 73

T

Temperature, rotational, 17, 73–75
Template effect, 44
Thermal energy, 14, 19, 84
Thermodynamic
 equilibrium, 26
Thermodynamic integration, 33, 35,
37–39
Thermodynamics, 1
Third law of thermodynamics, 89, 90
Trouton's rule, 106, 195, 201, 209

V

Van der Waals gas, 23
Volume
 cluster, 23, 24, 140, 141, 150–152, 160,
161, 204, 205
 excluded, 24, 25, 28, 160, 205
 free, 104, 108–116, 206
 translational, 84, 86, 104, 105, 109, 116,
117, 140, 159, 204, 205
Volume polynomial, 29

W

Wavelength, thermal, 15, 73, 74

Z

Zero point energy, 17, 49, 51, 52, 101