

Index

- ab initio* molecular orbital calculations, 137
ab initio prediction of crystal packing, 143–51
ab initio quantum-chemistry calculations, 119
 ABO₄ type structures, 257
N-(2-acetamido-4-nitrophenyl) pyrrolidine (PAN), 215–16
 acetic acid, 217
o-acetoamidobenzamide, 151–2
 acicular crystal, 101
 additives, enantiomeric distribution of, 188–90
 adiabatic processes, 14–15
 adjacency matrix, 229, 251
 ADP, 257, 298
 adjacency matrix, 244
 aqueous solution grown crystals, 306
 basic crystal graph, 246
 combinatorial properties, 243
 comparison of theoretical and experimental growth forms, 306–7
 conventional unit cell, 244
 crystal graph, 299
 crystal structure and bonds of first coordination sphere, 299
 derivation of the connected nets based on *f*, *g* and *h* bonds, 299
 energy computations of slices, 274–7
 interface behavior and surface–fluid interactions, 298–307
 results of sphere experiments and step-height measurements on pyramidal faces, 305–6
 structural morphology, 270–9
 theoretical growth form, 277–9
 aggregation/agglomeration, 107
 alanine, 169
 (R)-alanine, 220
 (R,S)-alanine, 210, 211, 212, 217, 221, 222
 alcohols, 120, 220
 aliphatic hydrocarbons, 120
 alkanes, 218
 allotropism, 320
 AM1 semi-empirical method, 141, 142
 amides, 123–5
 ammonia, 217
 ammonium chloride (NH₄Cl)
 F faces, 282
 fractal features, 283–4
 fractal growth pattern, 284
 gel-induced fractal habit of, 279–87
 growth units, 281
 octahedral habit modification, 287
 ammonium dihydrogen phosphate *see* ADP
 anthracene, 119, 127, 128
 anthranilic acid, 102
 anti-inflammatory steroids, 322
 area shape factor, 100
 aromatic hydrocarbons, 120
 aromatic size, 110
 asparagine, 176
 (S)-asparagine, 194–5, 207
 asparagine–aspartic acid monohydrate, 203
 atom–atom interactions, 118
 atom–atom method, 117–18
 atom–atom potential-energy functions, 168, 170
 atomic force microscopy (AFM), 168, 284
 atomic moments, 169
 atomic slice configurations, 275
 atropine, 328
 attachment energy, 126–7, 170, 207, 234
 azahydrocarbons, 120
 azobenzene, 111
 barite type structures, 257
 barium sulphate type structures, 251–6
 basic crystal graph, 242
 expressed as network, 243–6
 BCF model, 97
 BCF theory, 96, 97, 98
 benzamide, 113, 130, 131, 172, 173
 benzene, 341
 benzoic acid, 130, 131, 172, 173
 benzophenone, 111, 131, 132, 133
 benzoquinone, 116
 BFDH law, 102, 125, 235–6
 BFDH method, 104
 BFDH model, 126, 127
 bicyclohepta(*de,ij*)naphthalene, 144–5
 bicyclo(4.4.1)undecapentane, 139
 binary melting-point phase diagram, 328, 330, 332

- binding energy, 170
- birth and spread models, 96
- blocker additives, 131
- blocker molecule, 129
- boiling points, 133
- Boltzmann constant, 10
- Boltzmann distribution, 39, 41
- Boltzmann factor, 25, 38
- Boltzmann weighting, 25, 27
- bond energy, 289, 290, 295, 296
 - in organic molecular crystals, 320
- bond lengths, 141
- bonding, 71–3
 - “1–4”, 266
- Boyle temperature, 36
- Bravais–Friedel law, 102
- Bravais–Friedel–Donnay–Harker *see* BFDH law
- Bravais lattices, 58
- p*-bromophenyl acetic acid, 159
- Buckingham (B) potential, 32–3
- bulk diffusion, 97

- C* (end-centered) lattice, 59
- Cambridge Crystallographic Database, 108, 122
 - graphical input/output interface, 123
 - input query, 123
- Cambridge Structural Database, 320
- canonical distribution, 5
- canonical ensemble, 5, 7, 48
- carbon, 320
- carboxylic acid, 120, 123–5, 338
 - solid solutions of, 193
- carboxylic acid dimers, 111
- central-difference prediction, 52
- centrosymmetric crystals, 184–5, 216
- centrosymmetric space groups, 324
- centrosymmetric structure, 61
- CERIUS2, 104
- charge distributions, 24
- chemical bonds, 71–3
- chemical potential, 10, 20
- chiral additives, 213–14
- chiral compounds, solid forms of, 325–36
- chiral molecules, 324, 340
 - solid form of, 337
- chiral organic pharmaceuticals, solid-state
 - structure of, 313–45
- chiral selectivity, 176
- chiral shift reagents, 325
- chiral systems, polymorphic relationships in, 336
- chirality, 213–14, 313
- chlorpheniramine maleate, 338–9
- E*-cinnamide-2-*E*-thienylacrylamide, 196
- E*-cinnamic acid, 194–6
- close-packing arrangements, 337
- closed system, 9, 13
- cluster calculations, 340
- clusters, 92
- collision rate, 50–1
- combination of crystallographic forms, 98
- computational chemistry
 - crystal structure prediction/determination, 136
 - molecular materials, 106–65
- computer-based modeling methods, 1
- computer simulation, 1

- concept of microscopic reversibility, 41
- configuration integral, 34, 38
- configuration space, 38
- conformational isomorphism, 82
- conformational polymorphism, 79
- conformational symmorphisms, 82
- conglomerates, 334, 335
 - resolution by direct crystallization, 333
- connected nets
 - nets derived with *f* and *g* bonds taken into account, 301–4
 - nets derived with *f*, *g* and *h* bonds taken into account, 302–4
 - pictorial presentation, 301–6
- connectedness property, 242
- continuity equation, 3
- convergence, Madelung versus Ewald
 - formulations, 264–5
- Coulomb energy, 276, 282
- Coulomb interactions, 167, 168, 229, 260, 265–6, 277–9
- Coulomb potential, 260
- critical surface cluster size, 95
- critical transition supersaturation, 97
- crystal binding or cohesive energy, 118
- crystal chemistry of molecular materials, 108–17
- crystal dissolution, 174
- crystal energy, 234
- crystal engineering, 107, 111, 129, 170–4
- crystal faces, 98, 99, 101
 - attachment energy, 103
 - types, 103
- crystal form, calculation, 169–70
- crystal graph, 299
 - bipartite nature, 251
- crystal growth, 55, 89, 94–8, 166, 167
 - effect of solvent, 203–13
 - imperfect crystals, 96–8
 - inhibitors, 167
 - perfect crystals, 95–6
 - relay mechanism, 209–13
- crystal habit, 98, 99, 101–4
 - modification, 127–32
 - theory, 233
- crystal lattice, 56–9, 322, 338, 340
 - defects, 84
 - geometry, 125
- crystal morphology, 98, 127, 167, 168, 197, 237
 - effect of additives, 169–70
 - effect of solvent, 203–13
 - prediction, 293
 - quantitative determination, 169
 - simulations, 125
- crystal packing
 - ab initio* prediction of, 143–51
 - calculations, 135
 - Rietveld methods, 153–7
 - patterns, 146
 - problem, 149
- crystal planes (or faces), 98
- crystal shape, 98–102, 156
 - calculation, 125–7
 - and conditions of growth, 101
 - prediction, 125–31
- crystal structure, 102–4

- crystal structure (*cont.*)
 prediction/determination, computational chemistry, 136
 crystal surface, “tailor-made” additives on, 199–202
 crystal symmetry, 60–3
 lowering through additive occlusion, 199
 reduced, 188–98
 crystal systems, 58, 63
 crystal texture, “tailor-made” additives, 202–3
 CRYSTALDRAW, 279
 CRYSTALFORM, 279
 crystalline materials, 55
 crystalline phase formation, 213–22
 crystalline solid solutions, 82
 crystalline solvates, 205–7
 crystalline state, 55
 crystallization, 85–104, 330–2
 basics, 55–105
 bonds, 246
 direct, 332, 333
 crystallographic discrepancy factor, 122
 crystallographic forms, combination of, 98
 crystallographic point groups, 63–6
 crystallography, 323–5
 basic concepts, 55–84
 crystals, 55
 cubic lattice, 56
 cyanuric chloride, 117
- databases, 122–5
 Debye–Scherrer scattering geometry, 154
 deformation density maps, 168
 degeneracy factor, 5
 dehydroepiandrosterone (DHEA), 321–3
 diamond, 320
 diastereomers, 314, 316–19, 333
 dibromobenzene, 316
 6,13-dichlorotriphendioxazine, 154–7
 dielectric constant, 118
 4,8-dimethoxy-3,7-diazatricyclo(4.2.2.2-2,5-)
 dodeca-3,7,9,11-tetraene, 149–50
 dimethylsulfoxide (DMSO), 88
 dipeptide glycyl-glycine, 197
 dipleiadiene, 144
 dipole energy, 234
 dipole moments, 141
 Dirac delta function, 5
 direct chains, 247–8
 computation in terms of paths, 248–9
 computation of *F* slices in terms of, 249–50
 direct crystallization, 332, 333
 dislocations, 84, 96
 Disordered Flat (DOF) phases, 298
 dispersion contribution, 23
 dispersion energy, 27–8
 displacive transformation of secondary
 coordination, 75
 disrupter molecule, 129
 dissolution rate, 100
 Donnay–Harker law, 236
 donor–acceptor azobenzene, 108
 doublet, 239
- drug action, lock-and-key visualization of, 317
 drug development, 322
 dyestuffs, 120
- edge dislocations, 84, 85
 edge-to-face interactions, 127
 electric charge distribution, 24
 electric field, 268
 electrodynamic potential, 26
 electromagnetic forces, 22
 electrophotography, 106
 electrostatic contributions, 22–3
 electrostatic energy, 23–5, 168
 electrostatic interactions, 118, 222, 340
 electrostatic point charge model in PBC theory,
 260–5
 electrostatic potentials, 24–5
 enantiomeric distribution of additives, 188–90
 enantiomers, 314–16, 324, 325, 328, 330, 332, 333,
 338, 340
 resolution, 214–15
 enantiomorphism, 79–82
 enantiomorphous crystals, 220
 enantioselective adsorption, 222
 energy, long-range intermolecular forces, 23–8
 energy calculations, 168
 energy change by direct transfer, 16–17
 energy computations
 of ADP slices, 274–7
 in ionic structures, 260–70
 energy fluctuations, 10–11
 ensembles, 4
 enthalpy, 17–18
 entropy, 12
 epitaxial growth, 222
 equations of state, 20–1, 35
 equilibrium thermodynamics, 12–21
 ergodic theorem, 4
 Euler’s constant, 262
 eutectics, 328–32, 335
 Ewald formulation
 description of data, 268–9
 site potential for lamina shapes, 267–8
 Ewald method, 264–5
 exactly defined model, 1
 exponent of repulsion, 30
 external forces, work done by, 16
 external quantities, 9
- F* faces, 238
 ammonium chloride, 282
 analysis, 270–4
F lattice, 59
F slice cell, 248
F slices, 231–3, 238, 240–1, 258, 269–74, 283
 computation in terms of direct chains, 249–50
 determination, 237
 graph-theoretic approach, 242–3, 247–50, 257
 of gypsum adjacent to vacuum and water
 solution, 252
 ionic, 251, 256

- F* slices (*cont.*)
 profusion of, 256–7
 solution-activated, with irreducible borders in gypsum, 250–1
- F* subslices, 247–8
- face indices, indeterminacy of overall sign, 241–2
- feed-forward neural network, 133–6
- FFACE program, 259–60
- finite difference methods, 51
- first law of thermodynamics, 17
- first moment of charge distribution, 24
- first-nearest-neighbour interactions, 295–6
- first-nearest-neighbour models, 294, 297–8
 versus long-range models, 288
- flat faces, 103
- flat surfaces, 279–82
- flatness condition, 238
- Food and Drug Administration (FDA), 318
- FORTRAN, 42, 44
- fractal features of ammonium chloride, 283–4
- fractal morphology, 285
- fugacity, 8
- fullerenes, 320
- functional groups, 338
- garnet structure, 298
- gas particles, motion of, 33–4
- gel-induced fractal habit of ammonium chloride (NH₄Cl), 279–87
- Gibbs distribution, 5
- Gibbs free energy, 18, 19, 20, 89, 90, 92, 95
- Gibbs–Thomson equation, 92
- glide plane, 69
- glutamic acid, 176
- glyceraldehyde, 315
- glycine, 119, 176
- α-glycine, 175, 201, 204, 205
- γ-glycine, 216, 218
- glycyl-leucine additive, 197
- grand canonical distribution, 5
- grand canonical ensembles, 5, 8–10, 45, 47–8
- graphite, 320
- gravitational force, 22
- grazing-incidence x-ray diffraction (GID), 168, 199–201, 205, 218
- growth layers, 230, 238
 search procedures, 240–1
- GSTAT, 123
- gypsum
 adjacent to vacuum and water solution, 252
 morphology, 254
 solution-activated *F* slices with irreducible borders in, 250–1
- habit-controlling energy parameters, 233–5
- habit-controlling energy quantities, 266
- halocarbon propellants, 322
- halocarbon solvates, 322
- Hamiltonian, 1, 2
- Hankel function, 262
- hard-sphere (HS) molecules, 50–1
- hard-sphere (HS) potential, 29–30
- Hartman–Perdok theory, 103, 228–312
- HBD parameter, 136
- heat function, 17
- heat gained or lost, 16–18
- heat of formation, 141
- heat of sublimation, 133
- Heisenberg uncertainty principle, 5
- Helmholtz free energy, 10, 18, 19, 21, 34, 35
- hemihydrism, 313
- herringbone contacts, 198
- heterogeneous nucleation, 93
- hexafluoro-isopropyl, 218
- hexafluorovaline, 217
- hexagonal crystals, 98
- hexagonal systems, 66
- high-performance liquid chromatography (HPLC), 189
- high-pressure liquid chromatography (HPLC), 325
- high-resolution powder diffraction, 107, 154
- high-resolution synchrotron x-ray diffraction, 203
- homogeneous nucleation, 93
- hydrogen bond, 111–17, 120, 123, 136, 211, 229, 320, 337, 338
 distributions, 269, 277
- hydrogen-bonding potential, 118
- hydroxyurea, 320, 321
- hyoscyamine, 328
- I* (body-centered) lattice, 59
- i*–*j* interaction, 265–6
- i*–*j* pair, 265
- ibuprofen, 318, 325–7, 331, 332
- ICE9, 341
- ideal canonical ensemble, 21
- importance sampling method
 implementation of, 41–2
 theoretical background, 38–41
 variations, 42
- impurity effects, 130
- induction contributions, 23
- induction energy, 26–7
- inorganic materials, 166
- integral of interest, 37
- integral of motion, 4
- interatomic distance, 118
- intercell bonds, 245
- interfaces, actual bond energies, 289
- intermolecular bonding, 127
- intermolecular energy, 143
- intermolecular forces, 22–36, 193–8, 338
 sources of information, 33–6
- intermolecular interactions, 111
- intermolecular microscopic forces, 107
- intermolecular orientation, 25
- intermolecular potential, 35
 modeling, 28–33
- internal energy, 16–17, 19
 change in, 17
- interplanar distance, 238
- interstitial impurities, 84
- intracell bonds, 245
- inverse *n*-fold axis of symmetry, 61

- inverse symmetry operations, 324
 ionic bond energies, 296–7
 ionic bonds, 72
 ionic crystals, 228–312
 ionic graph, 251
 ionic structures, 229–31
 energy computations in, 260–70
 specialization to, 251–6
 ionization potential, 141
 irreversible processes, 14
 Ising model, 1
 Ising temperature, 289
 isomorphism, 82
- j*-subsystem entropy, 13
- K* faces, 232, 239
K slice, 239, 240
 KDP, 257, 270–9, 298
 aqueous solution grown crystals, 306
 comparison of theoretical and experimental
 growth forms, 306–7
 interface behavior and surface–fluid interactions,
 298–307
 results of sphere experiments and step-height
 measurements on pyramidal faces, 305–6
 kinetic crystallization, 332
 kinetic roughening, 291–2
 kinked faces, 103
- lactic acid, 315
 Laplace's equation, 262
 lattice energy, 133
 calculations, 108, 117–22
 versus crystal radii, 119
 versus sublimation enthalpy, 121
 lattice parameters, 56
 lattice planes, 66–8
 Laue method, 74
 law of entropy increase, 14
 Law of Successive Reactions, 78
 layer energy, 170
 Lennard-Jones atomic parameters, 275
 Lennard-Jones expression, 265
 Lennard-Jones molecules, 52
 Lennard-Jones potential, 31–2, 36, 51
 depth, 269
 function, 118
 (S)-leucine, 201
 Liouville equation, 3
 lock-and-key visualization of drug action, 317
 long-chain hydrocarbons, 218
 long-range interactions, 293–6
 long-range intermolecular energy, 27
 long-range intermolecular forces, energy, 23–8
 long-range models versus first-nearest-neighbour
 models, 288
- Madelung's equation, 263
 Madelung's formulation, 261–3
 Madelung's ion lines, 263
 Madelung's ion meshes, 263
 Maltese cross, 167
 Markov chain, 39
 ergodic, 40
 Maxwell–Boltzmann distribution, 8, 48, 53
 Maxwell–Boltzmann system, 20–1
 mean collision time, 50
 mean displacement, 42
 mean field theory, 296–7
 mean internal energy, 9
 mechanical invariants, 4
 mechanical quantities, 9
 melting point, 329–30
 metastable solutions, 87
 methanol, 206, 207
 (S)-methionine, 199–201
 2-methoxypyridine-1,4-dimer, 149
 Metropolis criterion, 41–2
 microcanonical distribution, 5
 microcanonical ensemble, 5, 7, 9, 13
 Miller indices, 66–8
 mirror plane, 61
 modeling intermolecular potentials, 28–33
 molecular chirality, 184–5
 molecular crystals, 72, 167
 molecular dynamics
 simulation, 48–53
 studies, 293
 molecular information, 136
 molecular interactions, quantitative estimates,
 168–9
 molecular materials
 computational chemistry, 106–65
 crystal chemistry of, 108–17
 molecular mechanics, 137–9
 simulation, 44–8
 within grand canonical ensemble, 47–8
 within *NPT* ensemble, 46
 molecular modeling, 1–54, 129
 molecular momenta, probability distribution for, 8
 molecular nuclei, 143
 molecular orbital methods, 140–3
 molecular slice configurations, 275
 molecular structure, 113, 154, 156
 calculation, 137
 molecular-structure/crystal-packing calculation
 algorithm, 137
 MOLPAK program, 146, 341
 monoclinic structures, 257
 Monte Carlo cooling approach, 147
 Monte Carlo method, 37–44, 158–9
 origin and fundamentals, 37–8
 simulation of molecular mechanics, 45–8
 Monte Carlo simulated-annealing process, 149
 MOPAC, 155
 morphine, 315
 motion of gas particles, 33–4
 multilinear regression analysis (MLRA) model,
 133–6
 multiplet, 239
 multistep transition probabilities of order *t*, 40

- naproxen, 334, 335
 neural networks, 132
 neutron diffraction, 196, 203
 next-nearest-neighbour interactions, 294–6
 $\text{NH}_4\text{H}_2\text{PO}_4$ *see* ADP
 nickel arsenide, 319
 nitrobenzene, 154
 noncentrosymmetric space groups, 324
 noncentrosymmetric structure, 61
 nonlinear optics, 190–1
 nonsteroidal anti-inflammatory drugs (NSAIDs), 317
 norfenfluramine dichloroacetate, 327
 normalization condition, 3
NPT ensemble, 46, 48
 nucleation, 89–93, 284
 early stages, 220–2
 theory, 91–3
 nucleation barrier, 213
 nucleation induction time, 91
 nucleation order, 93
 nucleation rate, 92–3
 nuclei formation, 92
NVT ensemble, 45
- N*-octylgluconamide, 208
 one-component graphs, 242
 one-dimensional Fourier series, 262
 open systems, 9, 19–20
 optical activity, 79
 optical birefringence, 192–3
 optical purification, 330
 optical purity, 325
 organic crystals, “tailor-made” etchants for, 174–6
 organic materials, 166
 organic molecules, 72, 108, 110, 133, 320, 338, 340
 orthorhombic crystals, 98, 99
 orthorhombic system, 68
 Ostwald’s step rule, 78
 over-the-counter (OTC) drugs, 318
 overlap forces, 22
 oxohydrocarbons, 120
- packing coefficient, 109–11, 337
 packing efficiency, 111
 packing potential energy (PPE), 133
 paclitaxel, 127, 129
 partial atomic charges, 275
 partial atomic point-charge sets, 277–9
 particle engineering, 107
 particle morphology, 107
 partition functions, 5, 8, 9
 Pauli Exclusion Principle, 22
 PBC theory, 102, 228, 230–7, 308
 electrostatic point charge model in, 260–5
 future work, 285
 graph-theoretic formulation, 242–60
 historical setting, 235–6
 morphological predictions, 283
 operational concepts, 237–42
 technical issues, 236–7
- PBCs, 102–3, 126, 242, 282
 additional, 237
 analysis, 127
 centrosymmetric structures, 236
 determination, 237
 direction, 236
 evidence for existence of, 231–3
 intersecting, 231, 236
 nonparallel, 238
- PCK83, 340
 periodic bond chain theory *see* PBC theory
 periodic bond chains *see* PBCs
 periodic boundary conditions, 49
 perylene pigment, 110–11
 perylenedicarboximide, 147–8
 pharmaceuticals, 313–45
 phase space, 2
 phase trajectory, 2
 phenylalanine, 205
 phosphorus, 320
 photodimerization, 196–7
 phthalocyanines, 106, 116
 planes of symmetry, 61, 62
 PLUTO, 123
 point-charge model, 260–5, 282
 point defects, 84
 point groups, 63–6
 point lattice, 57
 polar crystals, 177–84, 207–9, 216
 polar habits, 241–2
 polyethylene, crystal structure, 70
 polymer–polymer systems, 90
 polymers, 120
 polymorphic forms, 76
 polymorphic relationships in chiral systems, 336
 polymorphism, 74–9, 107, 215–20, 320, 322
 polymorphs, 320–2
 porphyrins, 116
 potassium chloride, solubility in aqueous solution, 87
 potassium dihydrogen phosphate *see* KDP
 potential energy of interaction, 73
 powder diffraction, 74, 154–7
 patterns, 152–9
 precipitation, 88
 pressure, 15–16
 primary nucleation, 91
 primitive (*P*) lattice, 58–9
 primitive lattice translations, 236, 240
 probability distribution, 40
 for molecular momenta, 8
 property estimation methods, 132–6
 proportionality relation, 289
 propylglucosamine, 335
 pseudo-Boltzmann factor, 46, 47
 pseudo-*F* face, 238
 pseudo-*F* slices, 238
 pseudo-flat surfaces, 279–82
 pseudorandom numbers, 43–4
 pseudotwofold symmetry interlinking hydrogen-bonded bilayers, 201
 pyridazino-(4,5)-pyridazine (PP), 143–4

- quartet, 239
 quartz crystals, 313
- racemic alanine crystals, 220–2
 racemic compounds, 330–4, 338, 340
 racemic crystals, 81
 racemic histidine, 215
 racemic mixtures, 80, 317, 322, 324, 325, 328–30,
 332, 334
 racemic switches, 318
 raffinose, 167
 random numbers, generation, 42–5
 random sampling procedure, 37
 random walk, 42, 43
 recrystallization, 332
 relative growth rates, 230–1, 233–5
 resolution, 330
 resorcinol, 208
 retinoic acid, 316
 reversible processes, 14, 15
 α -rhamnose monohydrate crystal, 206
 rhombohedron (*R*) lattice, 59
 Rietveld refinement method, 152–9
 Rietveld refinement program DBWS, 156
 rotational disorder transformation, 75
 Rough–Flat–Rough (RFR) kinetic phase
 transition, 292
 roughening, 289–93
 roughening models, 287–8
 roughening transition, 293–4
- S* faces, 232, 239
S slice, 239, 240
 Schrödinger equation, 27
 screw axis, 69
 screw dislocations, 84, 85, 96
 development of growth spiral, 97
 second harmonic generation (SHG), 190
 second law of thermodynamics, 14
 second moment of charge distribution, 24
 second virial coefficient, 35
 secondary nucleation, 91, 93
 selective solvent binding, 209–13
 semi-closed system, 9, 15
 semi-empirical quantum mechanics, 146
 shape factors, 100
 SHELXTL/PC, 157
 short-range interactions, 294–6
 silica, transformations of, 77
 single crystals, 107
 structure, 122
 structure analysis, 136
 study, 157
 x-ray diffraction, 122, 136, 155
 singlet, 239
 SIREN, 285
 slice energy, 126–7, 234, 266
 slices, 231–3, 238–41, 269
 classification, 238–9
 sobrerol, 334, 336, 337
 sodium chlorate, L and D crystals, 81
 sodium chloride, 61
 atomic arrangement, 61
 structure, 60
 sodium cyanide, 129
 sodium ibuprofenate, 332
 soft-sphere (SS) potential, 29–30
 solid form
 of chiral compounds, 325–36
 of chiral molecules, 337
 control, 322
 solid–liquid interface, 174
 Solid On Solid (SOS) model, 289–90
 solid solutions of carboxylic acids, 193
 solid-state chemistry, 107
 solid-state structure, 319–22
 of chiral organic pharmaceuticals, 313–45
 prediction, 336–42
 solubility, 86–7, 133
 Solution Induced Reconstructive Epitaxial
 Nucleation (SIREN), 279
 solutions, 86
 solvent–solute interactions, 101
 solvent–surface interactions, 203–5
 solvents, 86, 203–13
 role in crystal growth and crystal shape, 101
 space groups, 71, 324, 340
 spinodal curve, 91
 spinodal decomposition, 90
 statistical averaging, 3
 statistical distribution function, 3, 4
 statistical distributions, 2–3
 statistical equilibrium, 12
 statistical-mechanical theories, 293–4
 statistical mechanics, 2–11
 and thermodynamics, 9–10
 statistical methods, 132
 statistical weight, 12
 statistically exact information, 1
 steady-state condition, 40
 stepped faces, 103
 stereoisomerism, 313–19, 334
 stick and van der Waals (spacefill) representations,
 108
 stochastic matrix, 40
 stoichiometry, 328
 strong nuclear forces, 22
 structural morphology, 231–3
 ADP-type structures, 270–9
 sublayer roughening, 292
 sublimation enthalpy, 132–5
 subslice, 238
 substitutional impurities, 84
 β -succinic acid, 119, 127, 128
 sucrose, 167
 supersaturated solutions, 91
 supersaturation, 86–9
 supramolecular assemblies, 116
 surface diffusion, 96
 surface energy, 234
 SURFENERGY, 269–70, 275
 SURFGRID, 269–70
 SURFPOT, 269–70
 Sutherland (*S*) potential, 30–1, 36
 symmetry information, 136
 symmetry lowering, 186–202
 symmetry operations, 323–4
 symmetry roughening, 291
 synchrotron radiation, 218

- Synchrotron Radiation Source (SRS), 154
 synchrotron x-ray scattering, 199
 system temperature, 15
- t*-distribution, 37
 “tailor-made” additives, 168, 170, 171, 186–202, 216
 on crystal surface, 199–202
 crystal texture, 202–3
 “tailor-made” auxiliaries, 167
 “tailor-made” etchants for organic crystals, 174–6
 tartaric acid, 314, 316
 temperature, 15
 terephthalic acid (TPA), 88
 ternary solubility diagrams, 334
 tetragonal system, 67
 1,4,5,8-tetramethoxy-pyridazino-(4,5)-pyridazine (TMPP), 143–4
 theory of stochastic processes, 39
 thermal quantities, 9
 thermal roughening, 289–91
 thermally isolated system, 15
 thermochemical data, 132–3
 thermodynamic equilibrium, 15
 thermodynamic limit, 21
 thermodynamics
 and statistical mechanics, 9–10
 three laws of, 9
 thienylacrylamide, 196
 three-dimensional symmetry, 187
allo-threonine, 198
 (*S*)-threonine, 220
S-allo-threonine, 198
o-toluamide, 172, 173
p-toluamide, 172–4
 toluene, 131–3
 4-toluene sulfonyl hydrazine, 158–9
 transformations, 75
 of silica, 77
 transition matrix, 40
 transition probability, 40
 translational symmetry elements, 68–73
 transport coefficients, 48
 triclinic system, 67
 triethylammonium-6,7-benzo-3-*o*-hydroxyphenyl-1,4-diphenyl-2,8,9-trioxa-4-phospha-1-boratricyclo(3.3.1) nonane, 140–2
- trigonal systems, 66
 trimesic acid, 114
 2,4,6-trinitro-*N*-methyldiphenylamine (CSD), 146–7
 trivalent cations, influence on growth mechanism and morphology, 304–5
 twinning, 82–3, 220–2, 284
 two-dimensional crystal, 103
 two-dimensional Fourier series, 262
 two-dimensional surface nucleation, 95
 two-dimensional symmetry, 187
- ultraviolet irradiation, 214
 uniform sample mean method, 38
 unit cell, 56, 57, 125, 136
 dimensions, 144, 146, 154, 155
 urea, 119, 121, 213
- vacancies, 84
 vacuum sublimation, 157
d,l-valine hydrochloride, 338
l-valine hydrochloride, 338
 van der Waals energy, 276
 van der Waals equation of state, 36
 van der Waals forces, 337, 338
 van der Waals interactions, 114, 118, 119, 172, 229, 260, 265–6, 277–9, 288, 320
 van der Waals parameters, 168
 van der Waals radii, 114
 VISTA, 123
 volume shape factor, 100
- weak nuclear forces, 22
 WMIN, 340
 work done by external forces, 16
 Wulff form, 98–9
- x-ray crystallographic analyses, 319
 x-ray diffraction, 73–4, 196, 197, 199, 222, 319
 x-ray powder diffraction (XRPD), 324–5, 327
- zeroth moment of charge distribution, 24