

Index

a

- achiral helical arrangements
 - asymmetric units 274
 - mechanical constraints 276
 - $2n_H$ descriptors 273
 - poly(rA)-poly(rA) parallel double-helix 276
- achirotopic stereogenic carbon 114
- ‘acide racémique’ 47
- active pharmaceutical ingredients (API) 35, 200, 229
- adamantane-1-NMe₃ 264, 265
- AFMX four-spin system 210
- amorphous ‘frozen-liquid’ 53
- angiogenesis 28
- α - or β -anomeric configuration
 - furanose-ring anomeric hydroxyl group 64
 - L-galactopyranose 64
- antagonists 230
- Anti-Octant Rule 10
- antiperiplanar-type torsion angle 38
- API *see* active pharmaceutical ingredients (API)
- asymmetric carbon atom 113
- asymmetric unit
 - C₃-pseudosymmetric triangular array 150
 - crystallographic pseudosymmetry 149
 - diastereomers 151
 - dynamic disorder in crystals 222
 - multiple molecules 149
 - RMS superimposition values 151
 - (R)-symmetry cations 150
- atom flipping 222
- attention deficit disorder (ADD) 237

attention deficit hyperactivity disorder (ADHD) 237

Avnir CSM distortion indices 188

b

- Baeyer-Villiger oxidation 279
- Beer-Lambert law 70
- bioactive conformation 231, 232
- Biot’s law 45
- Bragg law 139
- Brazilian twin 55
- Brownian motion 165, 193
- Buscopan® 196
- ¹³C CP/MAS (cross polarization/magic angle spinning) pulse sequences 164

c

- charge coupled device (CCD) detectors 142
- chemical shift anisotropy (CSA)
 - line-broadening 193
- chiral axis 113
- chiral local site-symmetry 115
- chiral or asymmetric center 113
- chiral periodic arrays, *see also* periodic arrays
 - and chiral crystal array 134
 - *chiral space groups* 133
 - general position of symmetry 135
 - *high fidelity pseudosymmetry* 135
 - molecular structure 134
 - Pasteur’s crystallization 132
 - Sohncke space groups 133
- chiral plane 113
- chiral propellers 176
- chiral zero 33

- chirality, *see also* symmetry/
 - psuedosymmetry
 - achiral geometries 15
 - amino acid chirality 23
 - Cotton Effect's sign 10
 - drug therapy *see* drug therapy, chirality
 - extraterrestrial macro-scale chirality
 - – Jovian Great Red Spot 21, 22
 - – Martian dust devils 20
 - – *spiral galaxies* 20
 - – Venusian South Polar Giant Vortex 23
 - – gastropods 18
 - gustatory (taste buds) 26
 - olfactory receptors 26
 - pheromones 25
 - progestin norethindrone, first oral contraceptive drug 10
 - stereochemistry 10
 - structural property 9
 - symmetry vs. broken symmetry
 - – Gakuen Spiral Towers building 16
 - – Mercedes House 17
 - – golden ratio 16
 - tropical storms' tropicity 18
 - chiroptical properties
 - circular birefringence 68
 - circular dichroism (CD) 74
 - crystallography 74
 - enantiomer's configuration, gas phase 82
 - isomerism 67
 - Optical Rotatory Dispersion (ORD) 71
 - Chloride · Dihydrate quaternary ammonium salts 221
 - circular birefringence 45
 - *index of refraction*, concept 70
 - *in-phase* helical pathways 68, 69
 - monochromatic light source 69
 - *non-phase restricted* parallel helices 69
 - photon locations 69
 - quantum-mechanical phenomenon 68, 69
 - *symmetry mismatch* 70
 - circular dichroism (CD)
 - chiral medium 73
 - elliptical polarized light 73
 - molecular ellipticity 74
 - photon locations 72
 - cis-geminal coupling 107
 - complex multiplet 207
 - computer assisted drug design *see* x-ray crystallography
 - computer assisted molecular modeling (CAMM) *see* pharmacophore method, drug design
 - conformational searches 234
 - conformationally polymorphic crystals 232
 - constitutional isomers 67
 - contact time period 166
 - Continuous Shape Measures (CShM) 13
 - 'Continuous Symmetry Measures' (CSM) 13
 - Cotton Effect 71
 - Cotton Effect's sign 10
 - Coulomb explosion imaging (CEI) 82
 - cross polarization (CP) process 167
 - cross polarization/polarization inversion (CPPI) 194
 - cross-polarization (CP) 193
 - Crystal Structure Based Rational Design method 263
 - crystal, definition 148
 - crystallography
 - fractional coordinates 74, 75
 - hexagonal symmetry 77, 78
 - Miller indexes 75
 - rotational symmetry 76
 - Scanning Tunneling Microscope (STM) 74
 - cubane
 - adamantine, T_{CH} value 167
 - *Boltzmann distribution* of nuclei 165
 - cross polarization (CP) process 167
 - phase coherence 166
 - 'plastic crystals' 166
 - *radio frequency* (RF) 165
 - *relaxation mechanisms* 165
 - solid-state NMR spectroscopy 164
 - Curtin-Hammett principle
 - Z- α -benzamidocinnamic acid 106
 - CH₃ OC(=O)– methoxy carbon 108
 - chiral diphosphines 109
 - cis-geminal coupling 107
 - cis-hydrogenation, kinetically controlled 108
 - cyclopropyl analogue 105
 - diastereomeric transition-states 109
 - -menthyl/(-)-bornyl chiral ester substrates 104
 - methyl α -acetamidocinnamate, *re-si* prochiral face 106, 107
 - N-acetyl-(R)-phenylalanine ethyl ester product 110
 - ³¹P¹H NMR spectroscopy 106

- [Rh^I/(DIPHOS)]⁺. BF₄⁻π-complex bounding 110
 - (*R,R*)-trans-1,2-cycloalkyl analogues 105
 - slow magnetic site-exchange line-broadening 106
 - (*S,S*)-DIPAMP catalyst 109
 - stereogenic carbons 104
 - stereogenic phosphorus atoms 104
 - cyclononenes 214
 - cyclooctenes, olefinic stereochemistry 214
- d**
- Density Functional Theory (DFT) 79, 215
 - desymmetrization
 - Avnir CSM distortion indices 188
 - chemically significant divergences 188
 - chiral space group lattice 186
 - diffraction pattern 163
 - dirubidium closo-dodecaborate 163
 - distortion, Avnir CSM programs 161
 - dodecahedrane 162
 - *high symmetry* point groups 161
 - partial desymmetrization 163
 - platonic-solid geometry compounds 187
 - substituted Platonic-solid geometry molecules 188
 - symmetry equivalent methyl groups 186
 - *symmetry point group's order* 161
 - diamantane-4,9-di(NMe₃) 265
 - diastereomers 67, 115
 - dihedral angles
 - NMR data 34
 - torsion angles 35
 - 3,5-dimethyladamantane-1-NH₃ Cl 258
 - dipolar line-broadening 193
 - divalent anions
 - lobeline 189, 190
 - *hydrogen-bonding template* 191
 - monoammonium conformations 191
 - muscarine 189
 - nicotine 189
 - ring hydrogen-bonding pattern 190
 - dodecahedrane 145
 - desymmetrization 162
 - mobility 166
 - solids-NMR technique 164
 - dodecahedrane *see also* cubane
 - dopamine (DA) reuptake
 - cocaine
 - ammonium NH proton 242
 - aromatic ring centroid 241
 - axial NH back-bridged analogue 243, 244
 - equatorial NH 'front-bridged' 242
 - α-iso-pentyl methylphenidate-surrogate incorporation 252
 - non-N-methylated compound 252
 - ritalin's concentration 241
 - site pharmacophore 233
 - drug therapy, chirality
 - angiogenesis 28
 - clinical trials 30
 - electrostatic interactions 28
 - embryopathy 27
 - enantiomeric purity 27
 - ethical drugs 30
 - penicillamine 27
 - phocomelia 30
 - placebo effect 31
 - thalidomide 27, 29, 30
 - transcription 28
 - transcription factor 28
 - dynamic disorder in crystals
 - asymmetric unit 222
 - atom flipping 222
 - atom-flip BB/TCC dynamic conformational interconversion 228
 - lattice expansion 222
 - local magnetic fields 228
 - *gem-N,N*-dimethyl quaternary ammonium salts 222
 - medium rings, conformational interconversion mechanism 222
 - methohalide isostructural crystals 226
 - nefopam methohalide quaternary ammonium ions 223
 - non-quaternary and non-methyl suppression (NQS) partial spectrum 226
 - space filling 222
 - spin-lattice relaxation time constant 227
 - synclinal torsion angles 222
 - dynamic light scattering (DLS) 184
 - dynamic NMR (DNMR)
 - cyclohexane ring-inversion 94
 - diastereomeric C₂-symmetrical trans-1,2-dicholorocyclohexane invertomers 94
 - diastereomerization 95
 - diastereotopic anisochronous signals 90

- dynamic NMR (DNMR) (*contd.*)
- diltiazem · HCl, dissolution 97
 - enantiomeric cis-1,2-dichlorocyclohexane invertomers 94
 - ethyl-group diastereotopic methylene-protons 97
 - interaction distance 90
 - intrinsic diastereotopism 98
 - magnetic site exchange permutations 93
 - peak's line-width 90
 - rotamers 92
 - Slow Exchange Limit (SEL) 90
 - sterically-hindered bond-rotation 96
 - temperatures exchange rates 92
 - time scale 90
 - topomerization 93
 - variable-temperature 90, 91
- e**
- ebola virus 9
- ECD *see* electronic circular dichroism (ECD)
- electronic circular dichroism (ECD) 185
- embryopathy 27
- enantiomerization 94
- enantiomers 42
- enantiomorphous 50
- enantiotopic subunits, prochirality *see* prochirality
- end group modified retro-inverso (EGMRI) transformations 123
- endocyclic dihedral angles 219
- endocytosis 9
- β -endorphins 123
- ethano-bridge enantiomerization *see* T-symmetry chiral organic molecule
- ethical drugs 30
- exohedral guests 178
- f**
- fast magnetic site exchange broadening temperature conditions 181
- ferritin 185
- fragrances 26
- g**
- gas-liquid chromatography chiral columns 23
- golden ratio 1, 3, 16, 146, 147
- Group Theory 4
- ^1H CRAMPS (combined rotation and multiple pulse sequence 164
- h**
- helical stereochemistry
- B-DNA²³¹ 269
 - 3_1 screw displacement 271, 272
 - 3_2 spatial arrangement 272
 - translation and *rotation*, components 269
 - Z-DNA 269
- hemihedralism, crystalline tartaric acid salts
- ‘acide racémique’ 47
 - amorphous ‘frozen-liquid’ 53
 - chiral crystals, conglomerate 51
 - isomerism 47
 - molecular chirality 51
 - as mordant 46
 - optical activity 48
 - optical rotation and crystal properties 48
 - paratartaric acid 47
 - phenomenon of dissymmetry 53
 - polymorphism 49
 - sodium ammonium paratartrate 49
 - “Herkimer diamonds” 42
- high-fidelity pseudosymmetry 135
- concept of chirality 15
 - Continuous Chirality 13
 - Continuous Shape Measures (CSHM) 13
 - ‘Continuous Symmetry Measures’ (CSM) 13
 - *genuine symmetry, distortions* 13
 - pseudosymmetry fidelity 11
 - reflection symmetry 11
 - ‘Vitruvian Man’ 11
 - X-symmetry 13, 14
- homomers 67
- homotopic symmetry equivalent protons 215
- hybridization index 39
- hybridization of atomic orbitals 39
- i**
- integrins 8
- interferogram phenomenon
- *charge coupled device* (CCD) detectors 142
 - data measurements 141
 - diffraction pattern 140
 - *direct methods* 142
 - *final residual discrepancy index* or R-factor 143
 - Fourier transformation 140, 141
 - isotropic or anisotropic parameters 142

- iterative calculation process (*refinement*) 142, 143
- Karle-Hauptman *tangent formula* 142
- *phase problem*, X-ray crystallography 142
- *riding method* 143
- *sphere of reflection* 140
- intermeshing molecular helices
 - chemical constraint 287
 - dimer, complexes 288
 - electrostatic interaction 287
 - enantiomers' 286
 - Fe^{II} and Ni^{II} complexes 285
 - heterochiral and homochiral screws 282
 - homochiral intermeshing 289
 - inversion symmetry 287
 - Ir^{II} crystal structure 285
 - mechanical constraint 282, 287
 - Mn^{II} and Cu^{II} complexes 285
 - three-fold rotational symmetry 287
 - triple helices 283
- International Union of Crystallography 148
- isomerism
 - anisometric isomers 67
 - bonding parameters 68
 - diastereo-isomerism 68
 - *isometric isomers* 67
- isosteric replacements 251
- I-symmetry of viral capsids
 - asymmetric and chiral 7
 - capsid's structure 7
 - dissymmetric 9
 - ebola 9
 - function 8
 - *I-pseudo* symmetry 8
 - rod units 8

j

- J_{AX} and $J_{AX'}$ coupling constants 208
- J-coupling 207

k

- Karle-Hauptman *tangent formula* 142
- K_i concentration 239
- kryptoracemate chiral crystals
 - advantages of pseudosymmetry 154
 - higher order achiral crystals 153
 - *n-glide reflection pseudo* symmetry 156
 - P2₁ monoclinic chiral space group 153, 154, 159
 - pseudo-X diastereomers 152

- ring hydrogen-bonding pattern 154
- rmS(*inversion dislocation*) 156
- symmetry elements 156

l

- la Coupe du Roi
 - achiral
 - cis-3,7-dimethyl-1,5-cyclooctanedione (C_{2v}-symmetry) 279
 - Bürgenstock Conference on Stereochemistry 278
 - chemical relevance 281
 - chiral discrimination, observation 280
 - Plexiglas(Perspex) coupe du roi cubes 280
- Larmor frequencies 165
- 'lead nitrate thermometer' 200
- L-galactopyranose 64
- ligand exchange 113
- local environment effect, molecular structure
 - bioactive conformation 35
 - bonding parameters 34
 - computational models 35
 - crystal form, packing arrangement 35
 - dihedral angles 34
 - NMR data 34
 - time-averaged structures 34
 - X-ray crystallography 34
- local site-symmetry 114
- lysergic acid diethylamide (LSD) 233

m

- medium ring stereochemistry
 - 2,6-benzoxazonine compound, crystalline-state 218
 - butano-bridged epimeric cyclononene derivatives 213
 - cyclooctenes, olefinic stereochemistry 214
 - NMR structure determination
 - – antiperiplanar and synclinal vicinal protons 218
 - – antiperiplanar relationships 218
 - – broad-band proton decoupled 217
 - – crystalline N-desmethyl-2,6-benzoxazonine · HCl 217
 - – dihedral angles 220
 - – homonefopam analog 219
 - – N-desmethyl 2,6-benzoxazonine, twist-chair-boat(type III) conformation 220

- medium ring stereochemistry (*contd.*)
 - – nefopam · HCl 217
 - – solvated molecules 221
 - – vibrational frequency calculation 219
 - – *X-ray* crystallography 220
 - saturated 214
 - synperiplanar torsion angle constraint 214
 - transannular interactions 214
 - meso-cyclopropanes 114
 - methylphenidate
 - attention deficit disorder (ADD) 237, 241
 - attention deficit hyperactivity disorder (ADHD) 237, 241
 - axial N-methyl epimeric partner 244
 - binding affinity 240
 - cocaine 239, 240
 - equatorial N-methyl species 244
 - half maximal inhibitory concentration (IC_{50}) 239
 - hydrogen-bonding acceptor site 244
 - hydrophobic collapse phenomenon 246
 - K_i concentration 239
 - mirror symmetry 245
 - norepinephrine (NE) 237, 239, 250
 - ritalin 237, 239, 240
 - serotonin reuptake inhibitor (SSRI) drug 236
 - stress 236
 - Miller index 74
 - molar ellipticity coefficient 74
 - 'molecularly active' materials 44
 - molecular subunits, symmetry comparison
 - coded methane H-atoms 88
 - diastereotopic molecule 88
 - diastereotopism 89
 - isochronicity 87
 - racemic solvent 88
 - solvated dodecahedrane 87
 - solvent shell calculations 88
 - molecular symmetry
 - NMR anisochronism
 - – anisochronous signals 206
 - – D_3 -symmetry chiral diastereomer 205
 - – hydrogen-bonded
 - barbiturates/cyanurates 205
 - – hydrogen-bonding arrays 206
 - – rosettes 205
 - pattern recognition
 - – AFMX four-spin system 210
 - – digital resolution problem 207
 - – estimated standard deviation 207
 - – first order multiplet patterns 209
 - – homonuclear decoupling (HD) experiments 208
 - – inversion in transition order 211
 - – J_{AX} and $J_{AX'}$ coupling constants 208
 - – J-coupling 207
 - – multiple-intensity peaks 207
 - – non-symmetry equivalent coupling constants 209
 - – nuclear Overhauser effect (NOE) experiments 208
 - – number of transitions 208
 - – proton-proton vicinal coupling constants 207
 - 'molécules intégrantes' 44
- n**
- nefopam methohalide quaternary ammonium ions 223
 - nicotine 189
 - N-methylritalin crystals
 - compact epimeric diastereomer 247
 - dopamine reuptake inhibitor pharmacophore 248
 - nefopam methohalides 248
 - prototropic shift/nitrogen inversion 248, 249
 - static disorders in 246
 - non-symmetry equivalent coupling constants 209
 - Nuclear Magnetic Resonance (NMR) spectroscopy
 - coplanar arrangement 85
 - cubane 86
 - geminal and vicinal coupling 85
 - Karplus relationship 85
 - non-equivalent proton nuclei 85
 - Nuclear Overhauser Effect (NOE) intensity enhancements 37
- o**
- Octant Rule 10
 - octa-t-butyl-octasila-cubane 186
 - olefins, homogeneous hydrogenation
 - achiral gas chromatography 103
 - (RS,RS)-alkane racemic mixture product 102
 - Curtin-Hammett principle 104
 - dideutero-alkane, reductive elimination 102

- dihydrogen activation 103
- (*re-re*)-enantiotopic face 102
- trans-dideutero-olefin 101
- Optical Rotatory Dispersion (ORD)
 - achiral chromophore 72, 73
 - Beer-Lambert law 70
 - chiroptical data 71
 - circularly polarized photons 72
 - Cotton Effect 71
 - photon locations 71
- ORD *see* Optical Rotatory Dispersion (ORD)
- organic substances, structural representation
 - bonding geometries 57
 - cis-1,2-dimethyloxirane 63
 - configuration 59
 - dibromoethane 57
 - double-bond compounds 58
 - Dutch liquid 57
 - enantiomorphous orientation 63
 - ethanol 56
 - meso-tartaric acid 60
 - sodium ammonium paratartrate 55
 - staggered conformers 62
 - stereochemistry 59
 - sugars 60
 - tartaric acids 56
 - *X-ray crystallography* 59
- O-symmetry chiral molecules
 - atropisomeric edge-linkers 185
 - atropisomeric ligands 184
 - ferritin 185
 - X-ray structure determination 184

- p**
- partially modified retro-inverso (PMRI) 123
- $P2_1/c$, nature's favorite space group 153
- penicilliamine 27
- Penrose tiling matching rules 145
- periodic arrays
 - extended arrays/molecular crystals
 - – achiral space groups 127
 - – chiral and asymmetric units 129
 - – chiral space groups 127
 - – quazicrystals 127
 - – symmetry, general and special positions 130
 - – 'trivial' operations 129
 - – unit cell 127
 - general positions
 - – *cis/trans* core geometries 138
 - – molecular occupancy 136
 - – second order spin system 132
 - *special positions*
 - – first order splitting 131
 - – inversion symmetry 138
 - – molecular occupancy 137
- periodic lattice 44
- permutational isomers
 - aryl C(ipso) carbons 117
 - chemical shifts 122
 - exo/endo rotamers 117
 - graph theory 121
 - helicity 118
 - helicity interconversion 119
 - interconversion 122
 - one-ring flip diastereomerization mechanism 120
 - ortho edge-label exchange 119
 - orthogonal-ring hub transition state 119
 - polymorphous triarylamine crystals 117
 - residual diastereomers 122
 - 'standard dextro reference orientation' 119
 - standard orientation labeled 116
 - trialkylamines, pyramid geometry 117
 - triarylamine helicity interconversion 119
 - triarylamine propeller 121
 - triarylamines maximally stereochemically labeled 116
- pharmacophore method, drug design
 - active pharmaceutical ingredient (API) 229
 - artificial intelligence superimposition techniques 232
 - binding affinities 231
 - bioactive conformation 232
 - chemical groups, 3D arrangement 229
 - conformational searches 234
 - dopamine (DA) 233
 - drugs peripheral functionalities 229
 - energy conformer 231
 - nanomolar concentration therapeutic activities 231
 - neurotransmitters binding 229
 - pharmacophoric bioactive arrangement 232
 - pharmacotherapeutic agents 231
 - selective reuptake inhibitor (SRI) 230
 - steady-state neurotransmitter equilibrium concentration 230

- pharmacotherapeutic agents 231
- phase coherence 166
- pheromones 25
- phocomelia 30
- placebo effect 31
- 'plastic crystals' 166
- platonic-solid geometries *see* platonic-solid geometry hydrocarbons
- prochirality
 - double-bond faces 100
 - enantiotopic faces 100
 - prochiral descriptors 100
 - prochiral protons 99
 - *Re,si* descriptors 100
- progesterin norethindrone, first oral contraceptive drug 10
- Protein Data Base 291
- proton-proton vicinal coupling constants 207
- pseudoasymmetric carbon atoms 114
- pseudoscalar phenomenon 33
- pseudosymmetry *see* symmetry/pseudosymmetry
- pseudosymmetry emulation
 - Avnir *inv.exe* program 155
 - chiral crystal lattice 152
 - diphenhydramine derivatives 159, 160
 - *intermolecular pseudosymmetry* fidelity 151, 155
 - iron(II) complex 159
 - kryptoracemates 152
 - N-desmethylnefopam.HCl kryptoracemate molecules 156
 - *n-glide reflection pseudosymmetry* 156
 - $P2_1/c$, nature's favorite space group 153
 - pseudoglide or pseudoscrew-rotation 157
 - pseudoinversion symmetry 153
 - ring hydrogen-bonding pattern 154
 - rmS(inversion dislocation) 156
 - Second Kind, operations 152
 - *X-pseudosymmetry*, *rmS(X)* calculations 159
- q**
- quartz crystals hemihedralism
 - circular birefringence 45
 - D_3 chiral pseudosymmetry 43
 - D_{3d} and D_{6h} achiral symmetry 42
 - double-headed 42
 - 'enantiomorphism in quartz' 43
 - enantiomorphous 42
 - hemihedral faces 43
 - holohedral faces 42
 - optical rotation 45
 - subgroups 44
- quartz crystals, *u'*, *x'*-hemihedral faced right- and left-handed 54
- quazicrystal packing 146
- r**
- racemic compound crystal lattices 132
- refinement 142, 143
- retro-inverso (RI) isomers
 - *boat-boat* chiral conformation 124
 - end group modified retro-inverso (EGMRI) transformations 123
 - partially modified retro-inverso (PMRI) 123
 - peptide transformations 122, 123
 - pharmacokinetics 122
 - ring-chirality 124
 - stereogenic element 124
- rigid conformational analogue 232
- ritalin 237, 239, 240
- s**
- saturated medium rings 214
- sausage formulae, benzene six carbon atom 56
- Scanning Tunneling Microscope (STM)
 - Cu-surface electrode 81
 - Density Functional Theory (DFT) 79
 - desymmetrization 81
 - homochiral dimers 82
 - mechanical cleavage or electrochemical etching 78
 - molecular chirality 81
 - *organizational chirality* 79
 - pseudosymmetry 81
 - quantum mechanical phenomena 78
 - *quantum tunneling* 78, 79
 - symmetry relationship 74
- Scopolamine Hydrobromide
 - anhydrate and hydrated forms 201
 - API (active pharmaceutical ingredient) 200
 - Atropos Belladonna 191
 - Boehringer-Ingelheim and Phytex samples 199
 - bromide vs. chloride anions 202
 - Brownian motion 193

- conformational structure 194
 - CPPI (cross polarization/polarization inversion) 194
 - desolvated crystals 203
 - π -flip kinetic phenomenon 196, 197
 - and HCl salts 195
 - hydrogen-bond donors 203
 - *hydrophobic collapse* 195
 - magic angle spinning (MAS) 193
 - SELTICS pulse-program 198
 - single crystal X-ray diffraction 192
 - solid-state CP/MAS ^{13}C NMR spectroscopy 197
 - solid-state NMR spectroscopy 193
 - ‘trihydrate’ form 197, 200
 - variable amplitude cross polarization (VACP) pulse-program 198
 - SDRI *see* specific dopamine reuptake inhibitors (SDRI)
 - selectivereuptakeinhibitor(SRI) 230
 - SELTICS pulse-program (*side band elimination by temporary interruption of the chemical shift*) 198
 - single crystal X-ray crystallography *see* interferogram phenomenon
 - slow magnetic site exchange broadening temperature conditions 181
 - sodium ammonium paratartrate
 - double salt 51
 - hemihedral facets 49
 - sodium-D line 44
 - solid-state NMR spectroscopy
 - *chemical shift anisotropy (CSA) line-broadening* 193
 - *dipolar line-broadening* 193
 - solid-state *racemic compound* 132
 - specific dopamine reuptake inhibitors (SDRI) 244
 - back-bridged tropane derivative 250
 - C_α -alkyl ‘*methylphenidate-like*’ surrogates 250
 - DA/NE relative binding affinity 250
 - i-Pnt test compound 251
 - isosteric replacements 251
 - methyl branched-chain analogues 251
 - methylphenidate, branched-chain α -alkyl analogues 251
 - p-Cl aromatic ring substitution 250
 - spherical $(\text{CH})_n$ crystalline molecules *see* cubane
 - spherical $(\text{CH})_n$ crystalline molecules *see* dodecahedrane
 - spin-lattice time constant *see* time constant number one (T1)
 - spin-spin time constant *see* time constant number two (T2)
 - SRI *see* selective re up take inhibitor(SRI)
 - stereogenic elements 113
 - STM *see* Scanning Tunneling Microscope (STM)
 - Structure-Based Molecular Design technique 258
 - sweeteners 26
 - symmetry
 - dynamic stereochemistry 90
 - molecular subunits *see* molecular subunits, symmetry comparison
 - in NMR spectroscopy *see* Nuclear Magnetic Resonance (NMR) spectroscopy
 - symmetry arguments 33
 - symmetry molecules
 - chiral/achiral symmetry 171
 - crystal lattice 169
 - crystallization 169
 - duals in solid-geometry 170
 - O_h -symmetry, cube 171
 - symmetry/pseudosymmetry
 - apparent symmetry *see* high-fidelity pseudosymmetry
 - asymmetric vs. chiral *see* I-symmetry of viral capsids
 - chirality 9
 - ‘golden-ratio’ 1, 3
 - *Group Theory* 4
 - handedness or chirality 5
 - – chiral point groups 6
 - – First Kind 5
 - – Second Kind 5
 - ‘*high symmetry*’ 3
 - isometry 4
 - *point groups* 4
 - stone axe-heads, study 2
 - *symmetry operation* 5, 6
 - *symmetry transform* 6
 - *unit cell* 6
 - ‘*Vitruvian Man*’ drawing 1
 - synclinal torsion angles 222
- t**
- tartaric acid
 - isolation 45
 - molecular chirality *see* hemihedralism, crystalline tartaric acid salts

- tetradentate edge-linker units 183
 - thalidomide
 - adverse effects 30
 - advertisements 29
 - chirality, role 27
 - *over-the-counter remedy* 29
 - safety and effectiveness 30
 - time constant number one (T_1) 166
 - time constant number two (T_2) 166
 - topomerization 93
 - torsion angles and molecular conformation
 - anhydrate and monohydrate crystal structures 36
 - *boat-boat* conformation 37
 - bond angles 35
 - bond lengths 35
 - dihedral angles 36
 - molecule's environment 36
 - non-symmetry equivalent molecules 37
 - Nuclear Overhauser Effect (NOE) intensity enhancements 37
 - semi-quantitative descriptors 38
 - spatial arrangements 35
 - stereochemical terms 39
 - symmetry dependent 38
 - transcription factor 28
 - transmission electron microscopy (TEM) 184
 - triarylamine propellers 115
 - T-symmetry chiral organic molecule
 - ammonium ions 178
 - asymmetric unit building-block unit 176
 - chiral propellers 176
 - crystallographic T-point group symmetry 178
 - C_3 -symmetry 1,3,5-trisubstituted phenyl hexadentate ligands 180
 - D_2 symmetry 172
 - enantiomers 174
 - ethano-bridge protons 175
 - magnesium^{II} ions 176
 - molecular chirality 174
 - pseudosymmetry mimics 174
 - rhombohedral R3 chiral space group 173
 - spheriphane 175
 - synthesis 171
 - X-ray crystallography 174
 - T-symmetry clusters, enantiomerization
 - Bailar Twist 180
 - coplanar transition-state 181
 - diastereotopic methylene protons 181
 - energy of activation 182
 - twist-boat-chair (TBC) conformation 220, 221
 - cyclononane 214, 215
 - twist-chair-chair (TCC) conformation
 - atom flip 228
 - atom-flip dynamic interconversion 222
 - halide anion's van der Waal radii 222
 - temperature measurement 228
- v**
- Valence Shell Electron Pair Repulsion (VSEPR) paradigm 39
 - variable amplitude cross polarization (VACP) pulse-program 198
 - vibrational circular dichroism 82
 - vibrational Raman optical activity 82
 - 'Vitruvian Man' drawing 1, 11
- w**
- Watson and Crick's DNA model 144
 - Watson-Crick double helix 291
- x**
- x-ray crystallography 161
 - computer assisted drug design
 - – adamantane-1,3-di(NMe₃ I) 262
 - – asymmetric units 260
 - – avidin biotin complex 256, 257
 - – Avnir S(C7) parameter 260
 - – bonding and non-bonding interactions 263
 - – CB host 266
 - – C_7 pseudosymmetry 267
 - – *Crystal Structure Based Rational Design* method 263
 - – cucurbit[n]urils 257
 - – 3,5-diMe-Ada-1-NH₃ Cl composite 264
 - – electrostatic interactions 265
 - – ¹H NMR competition experiments 257
 - – memantine 259
 - – quaternary-NMe₃ salt 263
 - – sodium acetate-*d*3 buffer 258
 - – *Structure-Based Molecular Design* technique 258
 - – unused potential binding sites 255
 - X-ray diffraction
 - Bragg condition 140
 - by crystals
 - – aperiodic (quasicrystals) 139
 - – periodic (crystal lattice) 139

- - 'single crystals' 139, *see also*
interferogram phenomenon
- fiber diffraction
 - - B-DNA 143
 - - helical diffraction patterns 144
 - - *Patterson Function* 144
 - - Watson and Crick's DNA model 144
- x-ray fiber vs. single crystal diffraction models
 - DNA, dimensions and structural hypotheses 291
 - Protein Data Base 291
- 4_2 pseudo symmetry tetranucleotide duplexes 290
- Watson-Crick double helix 291
- X-symmetry
 - distance geometry algorithm 14
 - pseudo- and genuine symmetry 15
 - 'S(X)' CSM numerical index 13
 - - high-fidelity pseudo symmetry 15
 - - *integer number zero* 14, 15
 - - low-fidelity pseudo symmetry 15
 - - moderate-fidelity pseudo symmetry 15
- zero-point energy 40

