
Subject Index

Computer programs are denoted in boldface; databases and journals are in italics.

- Ab initio, 187, 194, 202, 210
Ab initio calculations, 47, 58, 59, 66, 87
Ab initio MO theory, 11
Ab initio model core potential (AIMP), 127
Ab initio VB theory, 2, 42, 45, 69, 84
Absolute configuration, 171
Absorption band, 164
Absorption spectra, 188
Acetaldehyde, 168
Acetone, 188, 191
Achiral, 65
Achiral chromophores, 203
Activation function, 254, 255
Activation value, 254
Activator variable, 225
Active bonds, 44
Active subspaces, 15
Active transport, 336
Acyl-CoA-synthetases, 334
Acytransferases, 334
Adaptive knowledge representation scheme, 263
Adiabatic approximation, 183
Adiabatic BO approximation, 171
Adiabatic profile, 51
Adiabatic reaction path, 102
Adiabatic states, 45
ADME/Tox (Adsorption, Metabolism, Distribution, Excretions, and Toxicology), vii, 333
Agglomerative clustering, 251
Alcohol-aldehyde dehydrogenases, 334
Alcohols, 75, 76
Algebraic methods, 249
Alignment independent QSAR, 347
Alkali dimers, 43
Alkanes, 49
Alkoxide anion, 75
Alkyl groups, 54
Alkyl radicals, 49, 62
Alkylhydrazine oxidase, 334
Allosteric behavior, 356
Allosteric effects, 369
Allosteric interactions, 356
Allyl anion, 57
Allyl cation, 57
Allyl radical, 57, 78
ALMOND, 347
Alzheimer's disease, 371
AM1, 187
Amide, 76
Amino acid sequence homology, 348
a-N₂O₂, 142
Analytical methods, 249
Angiotensin converting enzyme (ACE) inhibitors, 350
Annihilation operators, 178, 180
Annulenes, 59, 60
Anthracene, 164, 166, 205
Antianxiety molecules, 371
Antiaromatic molecules, 42
Antiaromaticity, 6, 12, 14
Antiarrhythmics, 365
Antibiotics, 379
Anticancer drugs, 363, 364
Anticooperative allosteric interactions, 356

Reviews in Computational Chemistry, Volume 20
edited by Kenny B. Lipkowitz, Raima Larter, and Thomas R. Cundari
ISBN 0-471-44525-8 Copyright © 2004 Wiley-VCH, John Wiley & Sons, Inc.

- Antidepressants, 371
Antipsychotic agents, 377
Antitargets, 338
Antiviral drugs, 363
Apical sodium-dependent bile acid transporter (ASBT), 351
Ar₅₄ cluster, 141
Ar-glyoxal system, 141
Atomases, 334
Aromatic compounds, 165
Aromatic molecules, 6, 9
Aromaticity, 14
Arrhythmias, 226
Artificial neural networks (ANNs), 254, 322
Ascorbate transporters, 361
Associative memories, 259
Atmosphere, 153
Atomic mean-field spin-orbit integrals (AMFI), 127
Atomic orbitals, 4
Atomic spin-orbit coupling, 106
Atoms in molecules (AIM) method, 76
ATP, 336
Aufbau principle, 10
Autocatalytic, 221, 241
Avoided crossing, 44, 45, 46, 48, 56, 57, 60, 61
Avoided crossings, 102, 129
Avoided surface crossings, 163
Axis switching effects, 174
Azidothymidine (AZT), 373
Azo and nitro reductases, 334
Azulene, 10, 165, 166, 198
- B3LYP, 187, 190, 191, 192, 193, 195, 204, 205, 207
B3LYP/SV(d), 195
B3LYP/TZV(d, p), 191, 192, 193, 200
Backpropagation, 254, 256, 257
Backward pass, 259
Bacteriorhodopsin, 353
Barbaralene, 64
Basis sets, 187
 aug-cc-pVQZ, 168
 aug-cc-pVTZ, 168
 aug-TZV(2df), 20
 6-311G(d, p), 135
 6-31G(d), 82, 13
 TVZ(2df), 200
 TVZ(d, p), 200, 202, 203, 205, 206, 209, 210
BEBO (bond energy bond order), 11, 84
Belief networks, 250
Belousov-Zhabotinsky (BZ) reaction, 219, 220, 226, 227, 233, 234, 235
Benzaldehyde, 164
Benzocyclobutendione, 164
Benzene, 6, 9, 20, 42, 57, 58, 59, 63, 74, 87, 180, 194
Benzene anion, 140
Benzene cation, 140
BERTHA, 132
BH, 132
BHLYP, 187, 190, 204, 207
Bile acid reabsorption, 351
Bile acid sequestrants, 351
Bile salt absorption, 351
Bimolecular reactions, 241
Binding energy, 29
Bioactive conformation, 344
Bioavailability, 335
Biorthogonal VB (bio-VB), 16
Bipyridine-ruthenium complex, 195
Bistability, 241
Bistable region, 220, 223, 233
 β -lactam antibiotics, 350, 363
Blood brain barrier (BBB), 335, 351, 355
Bohr, 307
Boltzmann distribution, 158
Bond angles, 5, 9
Bond diagrams, 21
Bond dissociation energy, 80
Bond lengths, 9
Bonding, 3
Boranes, 10
Born-Oppenheimer (BO) approximation, 101, 153, 162, 172
BP, 190
BP86, 190
Breast cancer resistance protein (BCRP), 364
Breathing orbital effect, 83
Breathing orbital VB (BOVB), 15, 16, 80, 81, 82, 83
Breit interaction, 116, 120
Breit-Pauli Hamiltonian, 120, 121, 124
Broken-symmetry artifact, 78
Bromate ion, 219
- C₃H₃[±] (cyclopropenium ions), 10, 39, 40,
C₄H₄ (cyclobutadiene, CBD), 6, 8, 9, 12, 19, 28, 32, 42, 57
C5, 164
C₅H₅, 6
C₅H₅[±] (cyclopentadienyl ions), 10, 39, 41, 42
C₇H₇, 6

- $C_7H_7^+$, 10, 39, 42
 C_8H_8 (cyclo-octatetraene, COT), 6, 8, 9, 42
CA rules, 228, 231, 232, 243
 Ca^{2+} waves, 226
Calcium channel modulators, 383
Cambridge Structural Database (CSD), 324
Canonical genetic algorithm, 265
Canonical MOs, 37
Canonical structures, 4, 7, 32, 33
Carbonyl group, 52
Carbonyl reductase, 334
Carboxyl group, 75
Carboxylate anion, 75, 76
Carboxylic acids, 75, 76
Cardiac tissue, 225
CAS (complete active space), 176, 178
CASMP2, 176, 180
CASPT2, 155, 176, 180, 188, 190, 191, 192, 195
CASSCF, 176, 180
Catalyst, 341, 343, 352, 357, 362, 374, 383, 387
Cationic drugs, 362
CatScramble, 343
CC stretching-bending mode, 197
CC2 (coupled cluster model), 164, 165, 176, 186, 202, 203
cc-pVDZ, 168
cc-pVQZ, 168
cc-pVTZ, 168, 186
CCS, 185
CCSD, 185
CCSDT, 185
cc-VDZ, 168
Cell membranes, 363
Cellular automata (CA), 221, 227, 228, 231, 232, 235, 238, 243
Cellular communication, 337
Cellular homeostasis, 337
Cellular membranes, 336
Central nervous system (CNS), 337, 353, 371
Cerius², 362, 374
 CH_3 , 140
 CH_3CON , 135
Chameleon oxidant, 84
Channels, 333, 336, 376
Chaos, 219, 233, 244
Chaos theory, 250
Charge-shift bonding, 44
Charge-transfer, 52, 54, 55, 62, 76
Charge-transfer excited state, 160, 161, 184, 187
Charge-transfer sensitizer, 195
Chebychev propagator, 142
Chem-X, 375
Chemical bond, 7
Chemical elements, 287
Chemical fronts, 224, 236, 242, 243
Chemical intuition, 317
Chemical patterns, 219, 223, 227, 231, 233, 234, 240, 243
Chemical rate laws, 240
Chemical reactions, 14
Chemical reactivity, 44
Chemical signaling, 226
Chemical turbulence, 236
Chemical waves, vii, 219, 220, 226, 228, 230, 243
Cheminformatics, 338
Chinoid structure, 198
Chiral molecules, 154, 170, 171, 200, 201, 204
Chiral resolution, 65
Cholestasis, 365
Chromophore, 64, 200
Cholesterol metabolism, 351
Circular dichroism (CD) spectroscopy, 155, 170, 171, 200, 201, 202, 204
CIS (CI singles), 165, 176, 178, 183, 186, 187, 205
CISD, 176, 178
CIS-MP2, 176, 178
Citric acid, 219
Classification, 323
 ClO_2 , 140
ClogP, 380
Closed-shell, 178
Closed-shell structure, 15, 36
CISO, 140
Cluster analysis, 273
Cluster shape, 274
Cluster validity, 274
Cluster visualization, 261
Clustering, 233
Clustering density, 261
Clustering methods, 249, 250, 251, 260, 263, 323
CMC, 339
CN, 12
CO, 12
Coarse grains, 221
Cognition, 268
Coherent control, 65
Collision induced intersystem crossing, 141
Columbus, 131

- Combinatorial chemistry, 366
CoMFA (Comparative Molecular Field Analysis), 344, 345, 355, 364, 367, 370, 371
Complete active space SCF (CASSCF), 72, 73, 82
Complete active space VB (CASVB), 14
Complex data sets, 263
Complex dynamics, 232
Complex network of reactions, 227
Complex phenomena, 221
Computational chemists, 11
CoMSIA (Comparative Molecular Similarity Indices Analysis), 346
Concurrent neuro-fuzzy models, 285
Condensed phases, 228
Condensed-phase spectra, 200, 201
Conductors, 78
Configuration interaction (CI), 17, 23, 25, 68, 74, 77, 78, 79, 108, 116, 121, 133, 176, 177, 178, 184, 185, 189
Configuration state functions (CSFs), 177, 180
Confirm, 341
Conformational analyses, 350
Conical intersection, 129
Conjugated polyenes, 14, 60, 62, 63, 65
Conjugated polymers, 138
Constitutive androstane receptors (CAR), 385
Continuously fed unstirred reactors (CFUR), 219, 234
Cooperative allosteric interactions, 356
Cooperative neuro-fuzzy models, 285
Core excitation spectra, 156
Correction rule, 257
Correlation consistent configuration interaction (CCCI), 72
Correlation diagrams, 5, 32
Correlation effects, 186
Correlation energy, 159
Cost function, 262
Cotton effect, 200, 201
Coulson, 7, 9
Coulson-Fischer (CF) wave function, 18, 20, 21, 23, 29, 30, 70, 77, 80, 87
Coumarin 102, 192, 193, 194
Coupled cluster (CC) methods, 176, 184, 186, 202
Coupled clusters - single and double excitations (CCSD), 83
Coupled map lattices (CML), 221, 232, 233, 234, 235, 236, 238, 243
Coupled-cluster theory, 116
Covalent bonding, 4, 5
Covalent structures, 12
Covalent-ionic superposition, 4, 5
Cr(CO)₆, 164
Creation operators, 178, 180
Crisp logic, 273
Crisp set, 269, 270
Criterion function, 251
Critical phenomena, 225
Crossing point, 46, 47, 55
Crossing probability, 110
Crossing seam, 109
Crossover rate, 266
CRUNCH, 15
Cubic lattice, 222
Cubic nullcline, 225
Cyclic adenosine monophosphate (cAMP), 226
2+2 cycloaddition reactions, 10
Cyclohexane, 157
Cyclopropyl radical, 62
Cyclosporin, 355, 356
CYP2C5, 348
Cytochrome P-450, 84, 334, 349, 365
Cytochrome P-450 3A4 (CYP3A4), 356, 384

D_{3h} structure of benzene, 62
D_{6h} geometry of benzene, 57, 58
Data mining, 263
Data representation, 273
Data visualization, 249
d-aug-cc-pVDZ, 189, 191
De novo molecule design, 338, 389
Decision, 249
Decision-making processes, 250, 268
Decoding function, 265
Defuzzification, 274, 284, 323
Degenerate molecular orbitals, 102
Delocalized BOVB (D-BOVB), 82
Delocalized nucleophile, 52
Delta rule, 257, 258, 259
Density functional theory, 11, 66
Density functional theory (DFT), 156, 157, 179, 180, 181, 182, 184, 187, 192, 195, 196, 203, 206
Density functionals, 188
Density matrix, 155
Density of states, 154, 163
Descriptors, 340
Dewar, 7, 9
Dewar resonance energy (DRE), 42
Dewar structures, 7, 74
Diabatic curve, 46, 48

- Diabatic state, 45, 80, 82
Diagnostics, 263
Diamagnetic, 35
Diatomic molecules, 154
Diborane, 5
Diels-Alder reaction, 10, 50
Differential dynamic correlation, 83
Diffuse functions, 168
Diffusion, 220, 238, 239, 242, 243
Diffusion coefficient, 221, 225
Diffusive coupling, 226, 233
Digoxin transport, 357
Dihydropyrimidine dehydrogenases, 334
DIM (diatomics in molecules), 11, 84
1,3-dimethylene-butadiene, 67
Dimerization of disilene, 50
Dimerization of ethylene, 50
Dipole moment, 154
Dipole operator, 171
Dipole polarizability, 182
Dipole-length form, 167
DIRAC, 131
Dirac equation, 115
Dirac Hamiltonian, 115
Dirac-Breit theory, 116
Dirac-Coulomb theory, 116
Dirac-Gaunt theory, 116
Dirac-Hartree-Fock, 116
Diradicals, 66
DISCO (DIStance Comparisons), 341, 343
DISCO features, 344
Discrete data set, 262
Disjoint clusters, 251
Dissimilarity functions, 252
Dissimilarity measure, 253, 263
Dissociation constants, 341
Dissociation energy, 72, 82
Distance-preserving projection method, 263
2,3-(S,S)-Dithiadecalin (DTD), 200, 201
Divisive clustering, 251
DK3 spin-free Hamiltonian, 127
Docking, 338
Douglas-Kroll transformation, 124, 126
Dragon, 374
Drug-enzyme interactions, 341
Drug candidates, 349
Drug absorption, 363
Drug development, 382
Drug discovery, 359, 370
Drug discovery screening, 370
Drug disposition, 356
Drug-drug interactions (DDI), 366, 391
Drug elimination, 363
Drug-ligand conjugates, 348
Drug-like molecules, 340
Drug metabolism, 337, 349, 367
Drug-receptor interactions, 384
Drug-transporter interactions, 349
Drugs, 349, 373, 376
Duschinsky effect, 174
Duschinsky transformation, 174
Dyes, 153, 192, 204
Dynamic electron correlation, 158, 161, 162, 178, 186, 192, 194
Dynamic spin polarization, 68
Dynamical electron correlation, 72, 77, 82, 83, 166, 130
Ecological modeling, 319
Economical analysis, 263
Effective core potential (ECP), 107, 122, 123
Effective core potentials (ECPs), 195
Effective Hamiltonian, 27, 28
Eigenfunction, 16
Electric dipole, 167
Electric dipole allowed transition, 170
Electrochemical gradient, 336
Electrochemical wave propagation, 225, 226
Electron affinity (EA), 184
Electron attachment, 51, 52
Electron correlation (EC), 82, 158, 159, 160, 161, 162
Electron density, 154
Electron detachment, 51
Electron pairs, 2, 3
Electron spin resonance (ESR), 8, 107, 140
Electron transfer, 51, 52, 78
Electronegativity, 107
Electronic spectra, vi, 153, 154, 155, 159, 163, 165, 178
Electronic structure, 47
Electronic transition, 168, 172, 173
Electronic wave function, 172
Electronically nonadiabatic processes, 101
Electron-nuclear interactions, 174
Electron-pair bonding, 2
Electron-transfer reactions, 143
Electrophile, 50, 51, 52
Empirical VB (EVB), 14, 84
Empty fuzzy set, 269
Enantiomers, 65
Endobiotic metabolism, 336
Endobiotic molecules, 335
Endothermicity, 46

- Enolate anion, 75, 76
Enols, 75, 76
Enzymatic, 15, 84
Enzymes, 143, 365
Epoxide hydrolases, 334, 370
Equation of motion (EOM) CCD, 143
Equation-of-motion coupled-cluster (EOM-CC), 154, 161, 185, 186
Error cost function, 253
Error function, 257, 262
Error minimization, 255
ESR g-tensors, 154
Ester, 52, 53
Esterases, 334
Ethene, 162, 170
Ethylene, 5, 67, 87
Euler scheme, 222, 224
Euler solution, 233
European pharmaceutical regulatory authority, 376
Evolution strategies (ES), 265, 266
Evolutionary algorithms, 264
Evolutionary programming, 265, 267
Exact Hamiltonian, 27
Exact HF exchange, 207
Exchange energy, 12
Exchange process, 56
Exchange-correlation potential, 182
Excitable behavior, 225
Excitable cardiac tissue, 228
Excitable dynamics, 226, 229
Excitable media, 225, 226, 228, 230, 231, 233, 243
Excitable wave propagation, 232
Excitation, 154
Excitation energies, 155, 164, 168, 169
Excited state, 225, 229
Excited state absorption (ESA) spectra, 198, 199
Excited state effects, 47
Excited state geometry optimization, 163
Excited states, 153, 154, 163, 167, 172, 174
Exothermicity, 46
Explicit scheme, 223
Extended Hückel theory, 29
Extinction coefficients, 171, 175
Eyring, 13, 44, 84

F₂, 43, 80, 82, 83, 141
F₂⁻, 43, 82
Facilitated transporters, 336
'Failures' of VB Theory, 34
Far from equilibrium, 219, 221, 232, 243
Feature extraction, 273
Feedforward NN, 254, 257, 264
Fermi golden rule, 110, 139
Ferrocene, 8, 10, 21, 164
Ferromagnetic bonding, 44
FH, 82
FHN kinetics, 242
Fine-structure splitting, 105, 122
Finite differences, 174, 222
Firing patterns, 259
Fitness evaluation, 267
Fitness function, 265
Fitness value, 264
FitzHugh-Nagumo (FHN) model, 225, 226, 227, 230, 240, 241, 242
Flames, 153
Flavin adenine dinucleotide (FAD), 143, 144
Flavin containing monooxygenase, 334, 372
Fluctuations, 221, 240, 242, 244
Fluorescence, 102
Fluorescent markers, 153
Fock operators, 179
Foldy-Wouthuysen transformation, 117, 120, 125
Forbidden transitions, 172, 173
Formaldehyde, 208, 209, 210
Formamide, 20, 77
Formyloxyl radical, 78, 79
Forward difference, 233
Forward pass, 259
Fourier transform ion cyclotron resonance (FT-ICR), 142
Fractional Factorial Design (FFD), 347
Fragment orbital VB (FO-VB), 21, 23, 37, 54, 55
Fragment orbitals (FOs), 19, 29, 87
Franck Condon (FC) approximation, 172, 173, 174, 194, 197, 207
Franck-Condon factor, 111
Franck-Condon overlap, 138
Franck-Condon-Herzberg-Teller (FC-HT) approximation, 173, 174, 206
Free energy of activation, 52, 53
Frontier MO theory, 10
Frontier orbital energies, 368
Fukui, 10
Full CI, 180
Funnel state, 102
Funnels, 14
Fuzzification, 283
Fuzzified information, 323

- Fuzzy 1-lines algorithm, 321
 Fuzzy associative memory (FAM), 324
 Fuzzy clustering, 273, 278, 306, 318
 Fuzzy c-means algorithm, 319
 Fuzzy controller, 282
 Fuzzy divisive hierarchical clustering (FDHiC), 304
 Fuzzy expert systems, 282
 Fuzzy genetic algorithms, 285
 Fuzzy graph pattern recognition, 320
 Fuzzy hierarchical characteristics clustering (FHiChC), 287, 304
 Fuzzy hierarchical cross-classification (FHiCC), 287, 297, 319
 Fuzzy horizontal characteristics clustering (FHoChC), 287, 305, 319
 Fuzzy inference rules, 283
 Fuzzy logic (FL), vii, 249, 269, 271
 Fuzzy multivariate rule-building expert system (FuRES), 323
 Fuzzy neural networks, 285, 322
 Fuzzy n-means (FNM) algorithm, 305
 Fuzzy optimal associative memory (FOAM), 324
 Fuzzy principal component analysis (FPCA), 278, 307, 313, 317
 Fuzzy processes, 269
 Fuzzy propositions, 271, 272
 Fuzzy quantifiers, 272
 Fuzzy reasoning, 269
 Fuzzy recognition, 318
 Fuzzy regression, 274, 276, 278, 321
 Fuzzy rules, 323
 Fuzzy set, 269, 283
 Fuzzy set theory, 252, 268
 Fuzzy subset, 270
 Fuzzy system, 269
 Fuzzy truth qualifier, 272

 Gallant pocket algorithm, 256
GAMSS, 131
GAMSS-UK, 15
 Gas-phase, 54
 Gas-phase spectrum, 158, 200, 201, 205, 207, 209
 Gastrointestinal (GI) tract, 348
 Gaunt interaction, 116
Gaussian, 15, 60
 Gaussian functions, 169, 206
Gaussian70, 11
 GeH₃, 140
 Genealogical table of elements, 304

 Generalized multistructure (GMS) method, 79
 Generalized perceptron, 256
 Generalized resonating valence bond (GRVB) method, 80
 Generalized valence bond (GVB) method, 11, 12, 15, 19, 35, 42, 70, 71, 75, 79, 80, 81, 82, 83
 Generalized valence bond perfect pairing (GVBPP) method, 70, 72
 Genetic algorithms, vii
 Genetic algorithms (GAs), 249, 250, 265
 Genetic operators, 265
 Geometry optimizations, 163
 Geometry relaxation effects, 165
 Glucuronic acid, 373
 Glucuronosyltransferases, 373
 Glucose oxidase, 144
 Glutathione, 375
 Glutathione S-transferases (GST), 334, 375
GOLPE (Generating Optimal Linear PLS Estimations), 346, 364, 371
 Gradients in concentration, 221
 Graham-Schmidt orthogonalization, 49
 Graph theory analysis, 320
GRASP, 387
GRID, 346, 347
GRIND (Grid Independent Descriptors), 347
 Ground state effects, 47
 Group orbitals, 20

 H₂, 17, 18, 21, 24, 43
 H₂⁺, 5, 24, 43
 H₃, 84
 Hansch-type QSAR, 355
 Hard computing, 250
 Harmonic approximation, 162, 172, 208
 Harmonic oscillator, 172
 Hartree-Fock (HF), 73, 74, 79, 82, 83, 158, 159, 178, 181, 182, 186, 189, 190, 194, 203
 HBr⁺, 132
 HCl⁺, 132
 Heavy atom effects, 132
 Heilbronner, 10
 Heisenberg, 1, 4, 14, 65
 Heitler, 4, 17
 Helicene, 202, 203
 Herzberg-Teller (HF) approximation, 173, 174, 208, 209
 Hessian updating, 128
 Hexatriene, 33, 68
 Hidden layer, 257

- Hidden nodes, 264
Hierarchical clustering, 251, 252
Hierarchical fuzzy classification, 293
High-dimensional data, 250, 260
High throughput assays, 382
High throughput screens, 367
HIV protease inhibitors, 383
HL (Heitler-London) wave function, 3, 4, 12, 20, 22, 23, 25, 86
Homology modeling, 340, 348, 367, 377
Homolytic bond breaking, 22
Homo-polar bonding, 4, 17
Hopf point, 226
Hopfield network, 259, 260
Hot-bands, 158, 206
HOTFCHT, 174
hPEPT2, 351
Hückel, 5, 7, 8, 14, 38, 39
Hückel $4n + 2$ rule, 6, 8, 39
Hückel MO (HMO) theory, 6, 7, 9, 13, 40, 41, 42
Human drug metabolism, 367
Human Ether-a-gogo Related Gene (hERG), 376
Human genome project, 337
Human Small Peptide Transporter (hPEPT1), 350, 351
Hund, 5
Hund's rule, 37, 68
Hybrid neuro-fuzzy models, 285
Hybridization theory, 4, 5, 11, 12, 16, 35, 37, 68, 73
Hydrogen abstractions, 49
Hydrogen atom, 168
Hydrogen atoms, 17
Hydrogen-bond acceptor, 343, 346, 352, 357
Hydrogen-bond donor, 343, 344, 352, 357
Hydrogen exchange reaction, 16, 50, 61, 78
Hydrolysis, 76
Hydrophobe, 343, 357
Hydrophobic centers, 344
Hydrophobic features, 352
Hydrophobic fields, 346
Hydrophobicity, 340
Hypercholesterolemia, 351
Hypervirial theorem, 167
Hypothesis Generation (HypoGen), 342, 343

IC₅₀, 341
Image processing, 263
Implicit solvers, 223
Imprecise data, 269, 284

Inactive subspaces, 15
Incomplete data, 261, 323
Indigo, 164, 192
INDO, 195
INDO/CIS, 139
Indole, 164
Inductive effects, 76
Inference rules, 273, 283
Information granularity, 284
Infrared (IR) spectroscopy, 320
Ingold, 7
Inhibitor variable, 225
Initial condition, 224
Insulators, 161
Integral membrane proteins, 336
Intensity borrowing, 174
Intersystem crossing, 103
Intersystem crossing rate, 138
Intrinsic membrane proteins, 353
Intrinsic reaction coordinate (IRC), 104
Intruder states, 187
IO, 132
Iodate-arsenous acid system, 223
Iodine-ferrocyanide-sulfite reaction, 219
Ion channels, 337, 376
Ionic (polar) bond, 4, 5, 10
Ionic structures, 9, 15
Ionization peaks, 39
Ionization potential, 52, 53
Ionization potential (IP), 156
Ionization spectrum of CH₄, 37
IR spectroscopy, 154, 163, 199
Isoelectronic series, 14, 56
Isoenzymes, 374
Isothiocyanate ligands, 196

Jablonski diagram, 102
Jahn-Teller distortion, 102
Jahn-Teller effects, 9, 13, 41, 42
Jet spectrum, 208

Kekulé structures, 6, 13, 42, 57, 58, 59, 62, 67, 73, 74, 87
Ketones, 188
K_i, 341
Klein-Gordon equation, 114
K_m, 341
K-means clustering algorithm, 251, 252, 262
Knowledge-based homology modeling, 353
Kohn-Sham (KS) DFT, 180, 183, 184

Labrynthine pattern, 219, 220, 225, 242
Lagrange multipliers, 128

- Landau-Zener Semiclassical Approximation, 111
- Langmuir, 3
- Lanthanide series, 316
- Laser dyes, 192
- Laser excitation, 65
- Lead optimization, 366
- Learning algorithm, 258, 323
- Learning rule, 262
- Learning theory, 250
- Leave-One-Out (LOO) cross-validation, 345, 347
- Lennard-Jones, 5, 12
- LEPS (London-Eyring-Polanyi-Sato), 11, 84
- Lewis, 2, 5, 20
- Lewis pairing, 12, 34
- Lewis structures, 36, 62, 77
- Li_2 , 43
- Li_2^+ , 43
- Limit cycle, 226, 227
- Linear combination of atomic orbitals (LCAO), 5
- Linear combination of VB structures, 75
- Linear least-squares regression, 321
- Linear projection methods, 252
- Linear separability, 255
- Linear-response (LR) methods, 154, 161, 178, 185, 186
- Line-broadening, 158
- Linguistic labels, 282, 285
- Local density approximation (LDA), 189
- Localized atomic orbitals, 16
- Localized bond orbitals, 10, 13, 37
- Localized nucleophiles, 52
- Localized-breathing orbital VB (L-BOVB) method, 82, 83
- London, 4, 13, 14, 17, 44, 84
- Longuet-Higgins, 7, 9
- Lorentzian functions, 207, 208, 209
- Lowest unoccupied MO (LUMO), 55
- Low-energy conformers, 341
- Low-spin states, 186
- Lukasiewicz logic, 271
- Macroscopic scales, 220
- Magnetic angular momentum, 112
- Magnetic dipole operator, 171
- Magnetic Hamiltonians, 65
- Magnetic transition moments, 155
- Magnetically induced CD, 171
- Main group elements, 11, 14, 16, 291
- Malonic acid, 219
- Mammalian transport proteins, 336
- Many-body interactions, 141
- Mapping procedures, 14
- Markov chain models, 220, 224, 238, 240, 242
- Markov processes, 220, 238, 239
- Mass action kinetics, 223, 240, 241, 244
- Matrix element, 11, 13, 37, 86
- Matrix-assisted laser desorption-ionization (MALDI) mass spectroscopy, 324
- MDDR*, 339
- Mean-field approximation, 179
- Mean-field spin-orbit method, 141
- Membrane-bound proteins, 337, 348
- Membrane penetration, 340
- Membrane permeability, 349
- Memorization, 260
- Mendeleev, 287
- Mesomerism, 7
- Mesoscopic models, 220, 221, 224, 237, 238, 242, 244
- Mesoscopic scales, 239
- Mesoscopic simulations, 240
- Metabolism, 390
- Metal-ligand charge transfer (MLCT), 196
- Metals, 161
- Metastable minimum, 108
- Metaxylylene, 67
- Methane (CH_4), 13, 20, 39, 73
- Methane cation (CH_4^+), 37, 38, 39
- Methyl chloride, 54
- Methyl transferases, 334
- Metric MDS, 253
- MgBr, 132
- Minimum energy crossing point (MEXP), 104, 128, 133, 136
- Missing data, 261
- MNDO, 187
- MNDO/CI, 187
- MO description, 22
- Möbius interactions, 39
- Model core potential (MCP), 124
- Modeling, 323
- Modified fuzzy regression, 277
- Molar extinction coefficient, 169
- MOLCAD**, 361
- Molecular dynamics, 220, 244, 353
- Molecular geometries, 5
- Molecular mechanics (MM), 15, 47
- Molecular orbital theory (MOT), v, 5, 7, 10, 11, 27, 30
- Molecular orbital-configuration interaction (MO-CI), 24

- Molecular oxygen, 143
Molecular properties, 140
MOLFDIR, 132
Møller-Plesset Second Order Perturbation Theory (MP2), 176, 185
Molpro, 15
Molybdenite (MoS₂), 291
Monoamine-diamine oxidases, 334, 370
Monoamine oxidase A, 371
Moore neighborhood, 231
Morphine, 373
Morse curve, 24
Most spin-alternated determinants (MSAD), 65, 67, 68, 69
MS-WHIM, 340
Mulliken, 5, 7, 8, 9
MULTICASE, 355
Multicomponent samples, 320
Multiconfiguration MM (MCMM), 16, 84
Multiconfiguration SCF (MCSCF), 71, 75, 79
Multiconfiguration VB (MCVB), 15
Multiconfigurational quasidegenerate perturbation theory (MCQDPT), 124
Multiconfigurational SCF (MCSCF), 116, 121
Multiconfigurational states, 161
Multidimensional scaling (MDS) methods, 253, 263
Multidrug resistance, 353
Multidrug resistance gene (MDR1), 337
Multidrug resistance protein (MRP), 337
Multilayer network, 254, 256, 257
Multilayer perceptron, 323
Multiple conformers, 343, 369
Multiple drug binding sites, 356, 384
Multiple pharmacophores, 384
Multireference coupled clusters (MR-CC), 175, 176, 185
Multireference configuration interaction (MRCI), 155, 176, 178, 179, 180, 185, 189, 191, 192, 196
Multireference MP2, 164, 176, 180, 185, 206
Multireference perturbation theory (MRPT), 154, 176, 180, 186, 189
Multireference states, 161
Mutation, 264, 266

N₂⁻, 132
Na₄, 164
N-Acetyltransferases, 334
Nanocrystalline TiO₂, 195
Nanoscales, 242
Naphthalene, 159, 166, 198, 199, 200

Near attack configuration (NAC), 84
Near-IR spectra, 324
Negative feedback, 221
Neon, 190
Neopentyl chloride, 54
Nerve tissue, 225, 226
Nested allostereism, 369
Neural fuzzy system, 284
Neural Network Research Center, 250
Neural networks, vii, 249, 250, 254, 256, 286, 380
Neuro-genetic systems, 286
Neuron, 254
Neurotransmitters, 372
New chemical entities (NCE), 349
Newton-Raphson procedure, 128
Newton's equations of motion, 220
Nitroxide group, 140
NMR, 154
NMR chemical shifts, 154
NMR shielding constant, 140
NO₂, 79
Noisy data, 323
Non-drug like molecules, 340
Nonadiabatic coupling matrix element, 103
Nonadiabatic processes, 102
Nonbonding interactions, 32
Noncircularly polarized light, 170
Nondynamical electron correlation, 72, 130
Non-linear kinetics, 221, 242, 243
Nonlinear projection methods, 253
Nonorthogonal orbitals, 75
Nonradiative decay, 102
Nonrelativistic electronic structure theory, 104
Nonrelativistic quantum mechanics, 112
Norbornene, 138
Normal modes, 172, 173, 174, 198, 206
Nuclear motion, 172
Nuclear wave function, 172
Nucleophile, 50, 51, 52, 53, 55
Nucleophilic attack, 52, 55, 76
Nucleophilic cleavage, 52, 53
Nucleophilic substitution, 51, 54
Nucleoside drugs, 363
Numerical methods, 249

O₂, 5, 35, 36, 37
Objective function, 262, 265
Octatetraene, 166, 206, 208
Octet rule, 2
o-Cyanophenol, 166
Off-line learning, 256

- Offspring, 266
Olefins, 54
Oligopeptides, 365
One-electron bond, 31
One-photon processes, 157
On-line learning, 255
Open gel reactor, 219
Open system, 221
Open-shell systems, 155, 160, 177, 196, 198, 200
Optical rotations, 154
Oral drug delivery, 349
Orbital angular momentum, 105, 112
Orbital selection rule, 55
Orbital size effect, 79, 83
Orbital symmetry, 14
Orbital-optimized multiconfiguration VB methods, 75
Ordered display, 261
Ordered groundwork, 261
Organic anion transporters (OAT), 363
Organic cation transporter (OCT1), 362
Organics, 155
Organometallic complexes, 21, 78, 83
Oriented media, 171
Orthoxyllylene, 67
Oscillations, 219
Oscillator strength, 168, 169, 170
Oscillatory dynamics, 226
Oscillatory media, 233, 243
Ostwald, 5
Outliers, 262, 322, 345, 347
Output value, 254
Overlap integral, 24
Oxidation of CO, 226
- P₄, 164
Paramagnetic, 5
Paramagnetism, 8
Paraxyllylene, 67
Pariser-Parr-Pople (PPP) method, 187, 199
Parkinson's disease, 371
Partial differential equations (PDEs), 230, 231, 232
Partial least square (PLS), 345
Partitional clustering, 251
Passive transport, 336
Pattern association, 323
Pattern formation, 228, 233, 236
Pattern recognition, 323
Pauli exclusion rule, 30
Pauli repulsion, 30
Pauling, 4, 5, 6, 9, 16, 37
Pauling's resonance theory, 7, 8
 π -Electron delocalization, 76
Penicillin, 324
Pentacene, 166
Peptide bond, 75
Peptidomimetic compounds, 350
Perception, 268
Perceptron, 254
Perceptron learning rule, 255
Perfect pairing approximation, 70
Perfectly paired wave function, 20
Pericyclic chemical reactions, 10
Perimeter model, 165, 205
Period-3 map, 234, 235
Periodic forcing, 234
Periodic table, 287, 307
Perturbation theory, 179, 186
Perturbation theory, 31
P-glycoprotein, 349, 353
Pharmacokinetic and pharmacodynamic (PK/PD) profiles, 349
Pharmacophore, 340, 351, 352, 357, 367, 377, 383
Pharmacophore alignments, 341
Pharmacophore generation, 341
Pharmacophore models, 341, 343, 369
Phase inversion rule, 62
Phase transition, 237
Phenol, 166
Phenothiazines, 355
Phenyl cation, 137
Phenoxy radical, 159, 196, 197, 198, 200
Pheromones, 320
Photochemical isomerization, 206
Photochemical reactions, 154
Photochemical reactivity, 14, 60
Photochemical studies, 163, 175
Photochemical synthesis, 153
Photochemistry, 65
Photocyclization, 62
Photodissociation dynamics, 141
Photodissociative branching, 133
Photoelectron spectroscopy (PES), 10, 13, 38
Piggybacking compounds, 349
Pigments, 192
Plasmas, 153
Platt nomenclature, 165, 205
PM3, 187
Polanyi, 13, 44, 84
Polarizabilities, 154

- Polarization functions, 4
Poling algorithm, 341,343
Poly(phenylenevinylene), 138
Polyamine oxidase, 334
Polyatomic molecules, 4
Polyenes, 66, 67, 68, 160, 165, 206
Pople, 11
Population analyses, 167
Porphyrin, 162, 164
Positive feedback, 221
Post-Hartree Fock methods, 127
Potassium channel, 376
Potential energy surface, 11, 78, 84
Precision, 249
Predissociation, 132
Pregnane X receptor, 349, 382
PRESS (Predictive Sum of Squares), 345
Principal component analysis (PCA), 252, 310, 347
Principal components, 253
Probabilistic reasoning, 250
Process control, 263
Projection methods, 250, 252
Projection operators, 38
Prostaglandin synthetase-lipoxygenase, 334
Proteins, 333
Protein crystallization, 353
Protein pockets, 14
Pseudo-Jahn-Teller effects, 9, 56, 57
Pyrene, 166
Pyridazine, 164
Pyrrole, 164
- QM(EVB)/MM, 84
QM(VB)-MM, 15
QM-MM, 15
QSAR, 340, 364
QSAR-2D, 374
QSAR-3D, 346, 367, 374
QSAR models, 339
QT interval, 376
Qualitative VB theory, 26
Quantum chemistry, vi
Quantum mechanical dynamics, 141
Quantum mechanics, 2
Quantum Monte Carlo, 175, 176
Quantum numbers, 3
Quasi-classical (QC) state, 24, 28, 29, 65, 87
- Radical additions, 54
Radical cleavage, 55
Radical reactions, 32, 48, 49
- Radicals, 160
Random phase approximation (RPA), 167
Random-walk models, 238, 239
Rare earth elements, 307
Rate constants for spin-forbidden processes, 110
Rate determining step, 52
Rate law, 225, 241
Rational design, 353
Reaction barriers, 14, 16
Reaction coordinate, 45, 52, 56, 63, 64, 80
Reaction kinetics, 223
Reaction rates, 223
Reaction trajectory, 55
Reaction-diffusion equations, 220, 221, 222, 223, 224, 225, 226, 228, 229, 232, 233, 243
Reaction-diffusion system, 234, 235, 237, 242
Reasoning, 268, 284
Receptors, 337, 382
Recognition, 260, 323
Recombinant CYPs, 367
Recombination, 266, 267
Recursive algorithm, 174
Reduced resonance integral, 29, 30
Reference wave function, 177
Refractory stage, 225, 226, 229, 230, 231
Regioselectivity, 44, 55
REL4D, 132
Relativistic effective core potentials, 123
Relativistic fine structure effects, 154
Reserpine, 355
Resolution of the Identity (RI) method, 185, 202
Resonance energy (RE), 3, 13, 31, 46, 48, 55, 79
Resonance hybrid, 7, 8, 76
Resonance integral, 25
Resonance mixing, 44
Resonance structures, 30, 79
Resonance theory, 3, 5, 6, 9, 10, 11, 39, 42
Resonating GVB (R-GVB) method, 79
Resting state, 226, 229, 230
Restricted active space (RAS), 176, 178
Restricted configuration interaction (RCI), 72
Restricted Hartree-Fock (RHF), 83
Restricted TDDFT, 197
RI-CC2, 186
Ring-aromatic features, 357
ROHF (restricted open-shell HF), 189
Rosenblatt perceptron, 255
Rotational modes, 172

- Rovibrational fine structure, 155
RRKM theory, 110, 138, 142
Rule of 5, 339
Ruthenium, 195, 196
Rydberg orbital, 189
Rydberg series, 157
Rydberg spectra, 155, 156, 188, 189
Rydberg state, 160, 161, 163, 184, 186, 187, 188, 200, 201
- Saddle point, 104
Sammon's mapping, 253
Sample function, 262
Scalar relativistic corrections, 121
Scattering theory, 157
Schlöggl model, 223, 224, 239, 240, 242
Schrödinger, 1
Schrödinger equation, 113, 177
Schrodinger's equations of motion, 220
Screening system for drug delivery, 350
SD (single and double excitations), 176, 177
Selection, 264, 266, 267
Self consistent field (SCF), 183
Self-organizing map (SOM), 249, 251, 259, 261, 262, 263
Self-replication, 232
Semibullvalene, 64
Semiconductors, 78, 161
Semiempirical methods, 165, 176, 187
Semiempirical MO methods, 9, 14, 58
Semilocalized AOs, 18
Semilocalized atomic orbitals, 15
Separability conditions, 255
Separation hyperplane, 255
Sequential regression process, 260
Si₂(CH₃)₆, 164
SiH₃, 140
Simulated annealing, 343
Simulating memory recall, 259
Single excitations, 160
Single nucleotide polymorphism (SNP), 376
Singlet coupling, 17
Site directed mutagenesis, 348
Size consistency, 175, 178
Slater, 6, 7
Slater determinants, 36, 160
SLC (SoLute Carrier), 337
Slime mould dictyostelium discoideum, 226
SIS₂, 140
Smart Region Design (SRD), 347
S_N2 reaction, 50, 51, 54, 55, 62
SNF 2.2.1, 174
Sodium Taurocholate Transporting Polypeptide (NTCP), 365
Soft computing (SC), 250
Soft computing techniques, 249
Solubility, 390
Solution, 54
Solvent, 14, 15, 51, 54, 158, 169, 200, 203, 237
 σ - π separation, 5
Spatial derivatives, 223
Spatiotemporal intermittency, 233
Spearman's rho ranking statistic, 357, 377
Speciation, 318
Speech recognition, 263
Spin angular momentum, 112
Spin contamination, 200
Spin density, 140
Spin exchange term, 24
Spin forbidden reactions, vi, 103
Spin matrices, 112
Spin multiplicity, 102, 103
Spin-allowed transitions, 158
Spin-coupled (SC) theory, 15, 19, 70, 72, 73, 75, 80, 81, 82
Spin-coupled valence bond (SCVB) theory, 74
Spin-eigenfunctions, 17
Spin-Hamiltonians, 65
Spinor, 112
Spin-orbit CI, 124
Spin-orbit coupling, 105, 123
Spin-orbit effects, 155, 196
Spin-orbit Hamiltonian, 106, 122
Spin-orbit matrix elements, 111
Spin-orbitals, 16, 84, 85, 86, 87
Spiral core, 231
Spiral wave, 219, 220, 226, 227, 230, 231
Spirals, 219
Split delocalized BOVB (SD-BOVB), 82, 83
Split localized BOVB (SL-BOVB), 82
Stability condition, 222, 233
State-averaged MCSCF (SA-MCSCF), 130, 132, 133
Static electron correlation, 158, 162, 194
Stationary point, 103
Steady states, 224
Steady-state concentrations, 223
Stereochemical predictions, 54
Stereochemistry, 46, 47, 54
Stereoselectivity, 44, 55
Stereospecificity, 55

- Steric bulk, 54
Steric effect, 54
Stiff differential equations, 223
Stochastic methods, 249, 265
Stochastic models, 240, 242
Stochastic rules, 221, 237
Strong orthogonality, 71
Structure-reactivity correlation, 52
Structure-reactivity model, 47
Styrene, 166
Subjectivity, 268
Sulfotransferases, 334, 372
Superconductivity, 13
Support vector machines (SVMs), 390
Surface of crossing points, 104, 128
SYBYL, 344, 361
Symmetric group methods, 15
Symmetry breaking, 79
Symmetry forbidden transition, 168
- Targeted delivery, 348
Taylor series, 172, 179
TDDFT-B3LYP, 157, 164, 200, 201, 202, 203, 204, 205, 206, 208, 209, 210
TDDFT-BHLYP, 204
TDDFT-BP86, 204
TeH, 132
TeLi, 132
Tetracene, 166
Tetrahedral intermediate, 52
Tetrazine, 157, 158
Text mining, 252
Theoretical electronic spectroscopy, 163
Therapeutic targets, 376
Thermochromism, 64
Thinking, 268
Thiocyanate ligands, 195
Thioformamide, 77
Thioindigo, 192, 193, 194
Thiopeptides, 76
Threading, 348
Three-electron bonds, 5, 8, 12, 14, 31, 35, 43, 62, 82, 83
Time dependent (TD) methods, 168, 176
Time-dependent density functional theory (TDDFT), 154, 159, 161, 164, 165, 176, 180, 181, 183, 184, 186, 187, 190, 191, 192, 193, 194, 195, 196, 197, 200, 205, 206, 208, 209
Time-dependent Hartree-Fock (TDHF), 167, 168, 176, 180, 181, 183, 184, 186, 187, 190, 194, 207
Time-dependent perturbation theory, 110, 165, 177
Time-dependent Schrödinger equation, 114, 133, 142
Topological descriptors, 351, 355
Toxicity, 319, 335
Toxicology end-points, 339
Toxicology models, 339
Training procedure, 255
Transition density matrix, 167, 170
Transition dipole, 168, 170
Transition dipole moments, 167, 168, 171, 172, 173, 174, 175
Transition metals, 14, 16, 155, 165, 187, 194, 291
Transition moment (TM), 154, 155, 157, 163, 165, 167, 174, 181
Transition probabilities, 165
Transition state, 22, 44, 46, 47, 55, 56, 58, 60, 61, 62, 63, 64, 101, 104
Translational modes, 172
Transporter modeling, 348
Transporters, 336
Tree searching, 320
Triage filters, 339
Trimethoxybenzoyloxyhimbine (TMBY), 355
Triplet coupling, 17
Tropone, 10
Truth values, 271
TURBOMOLE, 211
Turing machines, 228
TURTLE, 15, 16, 75
Twin-states, 60, 62, 63
Two-electron/two-center ($2e/2c$) bond, 16, 17, 19
Two-photon spectra, 157
- UDP-glucuronosyl-transferases, 334
Ultraviolet (UV) spectra, 320
Uniform crossover, 266
Unitary transformations, 13, 37
Universal computation, 228, 232
Universal fuzzy set, 269
Unpaired spins, 5
Unrestricted Hartree-Fock (UHF), 83
Unrestricted TDDFT, 197
Unstable state, 224
Unsupervised learning, 263
UTDDFT-B3LYP/cc-pVDZ, 199
UTDDFT-B3LYP/TZV(d, p), 197, 198
UV spectra, 155, 158, 169, 170, 171, 201
UV/visible light, 153

- Vague boundaries, 273
Val-bond, 16
Valence bond, 1,187
Valence bond configuration mixing diagram (VBCMD), 44, 45, 55
Valence bond correlation diagram (VBCD), 44, 50
Valence bond diagram, 58
Valence bond state correlation diagram (VBSCD), 44, 45, 48, 50, 51, 52, 54, 55, 56, 57, 58, 59, 62, 87
Valence bond theory (VBT), v, 3, 4, 7, 8, 10, 11, 13, 15, 39, 49
Valence bond-configuration interaction (VBCI), 16, 77, 78, 82, 83
Valence states, 188
Valence structures, 14
Validity functionals, 252
Van der Waals, 14
Van der Waals forces, 154, 158
Variable selection, 347
Variational methods, 177
Variational principle, 73
VB determinants, 17
VB diagram, 15, 35
VB structure, 37
VB wave functions, 16
VB2000, 15
VBHL (valence bond Heitler-London), 4, 5, 6, 7, 8, 9, 12
VBSCF (VB self-consistent field), 15, 75, 76, 77, 83
Vertical approximation, 163
Vertical electron affinity, 51
Vertical energy gap, 46
Vertical excitation energies, 165
Vertical ionization potential, 51
Vibrational effects, 155
Vibrational fine structure effects, 154, 167
Vibrational frequencies, 205
Vibrational induced broadening, 169
Vibrational modes, 172, 173
Vibrational normal coordinates, 172
Vibrational structure, 171, 204
Vibrational zero-point energies, 162
Vibronic coupling, 203
Vibronic structure, 174
Vibronic transition, 171, 172
Vinblastine, 356, 358
Vinblastine binding, 355
Vinyl group, 75
Virtual combinatorial library generation, 338
Virtual libraries, 340
Virtual orbitals, 77, 177
Visible absorption spectra, 157
Vision, 153
Visualization methods, 252, 389
Vitamin transporters, 361
Von Neumann, 227

Walsh diagrams, 8
Water, 158
Wave function, 3
Wave propagation, 223, 231, 240
WDI, 339
Wheland, 6
Woodward-Hoffmann Rules, 50
World War II, 7

Xanthine oxidase, 334
Xenobiotic metabolism, 336, 366
Xenobiotic molecules, 335, 353, 372, 373
Xenopus laevis, 226
Xiamen-99, 15, 16, 75
X-ray diffraction, 320, 323

Zadeh, 268
 Z^{eff} method, 121
Zero Point Energy (ZPE), 165
Zero-differential overlap approximation, 65
Zero-field splitting, 105