

Index

- ab initio calculations 34, 217, 227, 254, 268, 275, 280, 306, 311, 326, 336, 340, 361, 374, 383
- ab initio methods 311
- ab initio methods, CASPT2 338
- ab initio methods, CASSCF 34, 312, 343
- ab initio methods, CCSD 312
- ab initio methods, CEPA 313
- ab initio methods, CI 312
- ab initio methods, MCSCF 312, 343
- ab initio methods, MRD-CI 337
- ab initio methods, RASSCF 338
- ab initio methods, RASSI 338
- ab initio methods, SCF 312
- ab initio methods, SDCI 343
- absorbance 366
- absorption 377
- absorption coefficient 32, 57, 251, 272, 366, 379
- absorption coefficient, Planck mean 150, 158
- absorption coefficient, Rosseland mean 149
- absorption coefficient, harmonic mean 87
- absorption coefficient, straight mean 83
- absorption cross section 366, 374, 379
- absorption strength 328
- absorption, bound-free 223
- absorption, collision induced 76, 87, 91, 209
- absorption, continuous 223
- abundance, CNO 18, 31, 202
- abundance, circumstellar molecules 100, 116
- abundance, Fe 202
- abundance, solar 31, 202
- abundances 125
- active space 312
- adsorption 180, 187
- AlH 65, 386
- AIO 390
- AIO, dissociation energy 260
- ArH⁺ 415
- Arcturus 288
- asymptotic giant branch, AGB 2, 67, 71, 113, 164
- ATLAS 285, 287
- atomic line lists 282
- atomic lines 265, 282, 284, 287
- atomisation energy 254, 263
- band intensity 374
- band model method 80
- band strengths 308
- BaO 389
- barium stars 15, 18
- basis functions 339
- basis functions, Gaussian 311
- basis sets 314
- benzene, C₆H₆ 349
- BeO 388
- Berkeley Newsletter 398
- Berkeley program 44, 397
- BH 386
- BO 390
- BO₂ 389
- Boltzman factor 278
- Born-Oppenheimer approximation 274, 298, 311, 326, 339, 353, 378
- bound-bound transitions 267
- bound-free transitions 267
- branch 272
- bridged molecule 417
- brown dwarfs 61, 91
- C₂ 11, 40, 69, 73, 202, 282, 287, 399
- C₂, dissociation energy 253
- C₂H 43, 106, 129, 171, 227, 335
- C₂H, dissociation energy 253
- C₂H₂ 19, 40, 104, 143, 171, 182, 226
- C₂H₂, dissociation energy 253
- C₂H₃⁺ 427
- C₂H₄ 106, 347

- C_3 40, 106, 136, 363
 C_6H_6 349
 C_{60} 107, 176
 C_nH 114
 $C_{2n}H$ 136
 CaH 63, 386
 CaO 389
carbon chains, C_n 106, 136
carbon dwarfs, dC 61
carbon stars 6, 20, 33, 40, 69, 98, 101, 113, 134, 165
 CCN^+ 363
 CdH 388
CD-ROMs 285, 289
 CH 19, 47, 202, 241, 276, 282, 287
 CH , photodissociation 230
 CH^+ 205
 CH_2 362
 CH_2 , photodissociation 232
 CH_2^+ 332
 CH_4 31, 43, 84, 91, 105, 226
circumstellar chemistry 101, 119
circumstellar envelope 98, 113, 134, 226
circumstellar molecules 101, 114, 417
circumstellar shells, carbon-rich 102
circumstellar shells, oxygen-rich 108
 CN 11, 19, 20, 40, 86, 106, 242, 282, 287, 399
 CN , dissociation energy 260
 CN , red system 35, 204, 279
 CNC^+ 364
 CO 11, 19, 31, 84, 104, 114, 171, 201, 242, 282, 287
 CO , photodissociation 227
collision induced absorption, CIA 63, 76, 87, 91, 209
collision induced dipole 209
collision rates 237
collisional processes 22
column density 100, 121
complete active space SCF, CASSCF 312, 343
configuration interaction, CI 268, 312
configuration interaction, SDCI 343
continuous absorption 223
continuous opacity 215, 216, 223
convection 58
cooling function 94
coupled-electron pair approximation, CEPA 313
critical cluster 172
cross section 226
cross-section, collisional 22
cross-section, dissociation 22
cross-section, ionization 22
 CS 32, 41, 105
 CsH 385
 CuO 392
cyanopolyynes, HC_nN 114
cyanopolyynes, $HC_{2n}CN$ 135
degenerate matter, equation of state 72
destruction rate 236
diatomic molecules 196
dielectric function 153
dielectric mirrors 371
diffusion approximation 266
dipole moment function 297, 360, 412
dipole transition 271
discrete variable representation 298
dissociation energy, determination of 254, 255, 262
dissociation energy 20, 35, 199, 224, 250
dredge-up 4
dust 54
dust, se also grains
dust, carbon-rich 99
dust, circumstellar 100, 143, 165, 171, 187
dust, interplanetary 188
dust, interstellar 187
dust, models 188
dust, molecular cloud 188
dust, opacity 186, 194
dust, oxygen-rich 99
dust, primary components 163, 171
dust, protostellar 188
dust, spectral characteristics 176, 190

- dye laser 370
dynamic correlation 341
effective temperature, T_{eff} 30
Einstein coefficient 317, 378
electric dipole moment function 311
electric discharge 412
electron correlation 312, 341, 343
Elsasser model 81
emission 377
emissivity 265
energy release from chemical reaction 255
enthalpy of formation 250, 261
equation of state 266
equilibrium constants 199
excitation temperature 119
extreme non-local thermodynamic equilibrium, XNLTE 186
FCI benchmark calculations 312
FeH 43, 59, 65, 198, 323, 388, 403
FeO 391
finite basis representation 298
fluorescence, laser induced 256, 367
flux 57
flux, continuum 13
Fourier transform spectroscopy, FTS 109, 401, 412
Franck-Condon approximation 378
Franck-Condon factor 85, 320, 378, 407
Franck-Condon principle 328
free-free transitions 267
freeze out model 101
fullerenes 107, 176
GeH 387
gf-value 9, 275, 282, 318
grains 114, 122, 125, 149, 163, 186
grains, se also dust
grains, SiC 143
grains, absorption 152
grains, carbon 100, 106, 143, 154, 159, 188, 191
grains, charged 181
grains, chemical growth 181
grains, chemical reaction network 174
grains, coagulation 182, 193
grains, continuous distribution of ellipsoids (CDE) 152, 155
grains, destruction 163, 192
grains, dirty ice 188, 193
grains, equilibrium 150
grains, fractal structure 182
grains, fragmentation 193
grains, graphite 155, 182, 191
grains, growth 173, 178
grains, heterogeneous 166, 180
grains, homogeneous 166, 180
grains, iron 154
grains, optical properties 154
grains, shape effects 155
grains, silicate 100, 108, 154, 158, 177, 191
grains, silicon carbide (SiC) 154
grains, size distribution 151, 170, 178, 183, 187
grains, surface chemistry 188
 H^- 39
 H_2 31, 74, 87, 91, 103, 214, 240, 282, 287
 H_2^+ 76, 215
 H_2C_n 114
 H_2F^+ 364
 H_2O 19, 37, 63, 84, 108, 114, 287, 296, 299, 362, 366
 H_2O , blanketing 57
 H_2O , photodissociation 229
 H_2O^+ 335
 H_2Se 363
 H_3^+ 76, 223
H2-H2 opacity 219
H2-He opacity 219
harmonic oscillator 354
harmonic oscillator approximation 367
HCN 19, 40, 84, 104, 143, 296, 306,
HCN, dissociation energy 263
HCN, overtone spectrum 373
 HC_nN 114
 HC_{2n}CN 135
 HC_{2n}H 136
HCO 328

- Herman-Wallis effect 415
 Herriott cell 368
 HgH 388
 HITRAN data base 93, 300
 HNC⁺ 364
 HNC 306
 HNSi 364
 HO₂ 364
 hot bottom burning, HBB 7
 HOC⁺ 363
 Hönl-London factor 274, 277
 hydrocarbon C_nH 114
 hydrocarbon chains, HC_{2n}H 136
 hyperfine structure 336
 ices 108
 infrared arrays 109
 integrated absorption coefficient 360
 intensity 226, 265, 272, 377
 intensity, band 374
 intensity, line 82, 297, 360
 intensity, measurement 382, 415
 intensity, specific 235
 interstellar molecules 417
 interstellar radiation field 226
 intracavity loss absorption spectroscopy 370
 IRC+10216 101, 114, 134, 136
 isotopic ratios 126, 203
 Just Overlapping Line Approximation, JOLA 87
 KH 385
 KO 388
 Klein-Dunham potential 277
Λ-doubling 272
 LaO 3, 44, 391
 laser gain bandwidth 370
 laser induced fluorescence, LIF 256, 367
 laser photofragmentation 262
 laser vaporization 257
 lifetime 376, 380
 lifetime, measurements 382
 LiH 24, 384
 line identification 197
 line intensity 82, 360
 line separation 82, 85
 line strength 274, 278, 318, 360
 LiO 388
 LiOH 364
 local thermodynamic equilibrium, LTE 22, 186, 196, 235, 265
 long-path spectroscopy 367
 Lyman alpha satellites 75
 M dwarfs, dM 49, 61, 92, 302
 M stars, parameters 49
 M stars, pressures 50
 M stars, spectra 58
 M stars, temperatures 52
 M stars 2, 33, 37, 49, 98, 165, 296
 M sub dwarfs, sdM 61
 masers 116
 mass loss 72, 99, 113, 120, 137, 164, 171
 matrix elements 345
 mean line separation 83
 metallicity, *Z* 30
 MgH 18, 63, 282, 287, 386
 MgO 171, 329, 388
 MgS 146
 Michelson interferometer 401
 Mie theory 152, 156, 190
 millimeter wave spectroscopy 417
 Mira variables 59
 mixing length theory 74
 MnH 388
 model atmospheres 29, 149, 200, 223, 286, 303
 model atmospheres, classical 93, 95, 235
 model atmospheres, extended 50
 model atmospheres, grids 289
 model atmospheres, multiple solutions 58
 model atmospheres, program 289
 model atmospheres, sphericity effect 90
 molecular beams 256, 262
 molecular clouds 188, 190
 molecular constants 35, 203
 molecular equilibria 55

- molecular formation and destruction 234
- molecular ion 417
- molecular line lists 279
- molecular line lists, HITRAN 93, 300
- molecular line lists, SCAN 34
- molecular line lists 29, 282, 318, 397, 409
- molecular lines 417
- molecular orbitals 311
- “molecular regime” of stellar parameters 30
- molecule fixed axis system 355
- molecule-grain transition 166
- monohydrides 384
- monoxides 384
- MORBID 35, 354
- Morse potential 277
- multi-configuration SCF, MCSCF 312, 343
- multi-configuration methods 343
- multipass cell 367
- multireference configuration-interaction method; MRD-CI 337
- N_2 11, 32
- N_2^+ 414
- N_2O , dissociation energy 262
- NaH 26, 385
- NaO 388
- $NC-CN$, dissociation energy 261
- net flux 265
- neutron source 6, 18
- NH 19, 202, 282, 287, 414
- NH , photodissociation 231
- NH_2 364
- NH_2^+ 363
- NH_3 31, 105, 226
- NO , dissociation energy 252
- non-adiabatic interaction 329
- non-local thermodynamic equilibrium, NLTE 22, 186, 223, 235, 266
- non-thermal velocity 93
- nucleation, classical theory 176
- nucleation, heterogeneous 178
- nucleation, homogeneous 177
- nucleosynthesis, $^{13}C(\alpha, n)^{16}O$ 7, 18
- nucleosynthesis, $^{22}Ne(\alpha, n)^{25}Mg$ 6, 18
- O_2 , dissociation energy 253
- O_4^+ 349
- OH 19, 32, 114, 200, 202, 282, 287, 314, 411, 414
- OH , photodissociation 229
- opacity data 159, 269, 282
- opacity distribution function, ODF 87, 282, 285, 289, 297
- opacity effects 55, 58
- opacity errors: effects on structure 55, 58
- opacity sampling, OS 87, 159, 268, 287
- opacity sources 322
- opacity, H_2-H_2 214, 219
- opacity, H_2-He 214, 219
- opacity, Rosseland mean 266, 286, 288
- opacity, atomic 265, 269
- opacity, collision induced 63
- opacity, continuous 37, 63, 215, 216, 223
- opacity, molecular 234
- opacity, monochromatic 270
- optical cavities 368
- optical depth 235, 265
- oscillator strength 10, 85, 226, 238, 251, 272, 275, 318, 327, 345, 376, 379
- overionization 240, 245
- overtones 367
- Padé approximant 311, 318
- partition function 35, 59, 199, 250, 267, 278, 360
- PbH 387
- perturbation 380
- perturbation expansion 297
- photoacoustic spectroscopy 369
- photodissociation 101, 117, 140, 223
- photofragmentation, laser 262
- photoionization 101
- Planck function 235, 238

- Planck mean absorption coefficient
150, 158, 159
- planetary nebula, PN 71, 100, 113,
134
- polarizability 153
- polyatomic molecules 245
- polycyclic aromatic hydrocarbon, PAH
107, 134, 140, 175, 178, 181
- polyynes 135, 137
- population III stars 215
- post-AGB objects 128
- potential energy function 228, 276,
298, 326, 339, 353, 412
- pre-planetary nebulae 134
- predissociation 224, 317, 380
- pressure induced absorption 209
- production rate 236
- protostellar objects 186, 188, 190
- radiation field 234, 238
- radiative lifetime 280, 320
- radiative processes 22
- radiative rates 238
- radiative transfer 56, 235, 246, 265
- radicals 136, 412
- random band model 81
- rate constant, C_i ; 22
- Rayleigh scattering 153, 215
- reactive species 417
- red giant branch, RGB 71
- reference configuration 355
- refraction, index of 153
- regular band model 81
- relativistic effects 317
- R-matrix methods 268
- Renner-Teller effect 333
- Rosseland mean absorption coefficient
149, 159
- restricted active space SCF, RASSCF
338, 344
- restricted active space state interac-
tion, RASSI 338, 345
- rigid molecule 354
- rigid-rotator-harmonic-oscillator 84
- ring-down cavity spectroscopy 371
- ro-vibrational bands 317
- rotation spectra 198
- rotation-vibration spectra 198
- rotational line 271
- rotational spectrum 417
- rovibrational coupling 297
- Rydberg states 328
- Rydberg-Klein-Rees potential, RKR
276
- SCAN-CN 35, 279
- scattering coefficient 57
- scattering 267
- ScH 387
- Schrödinger equation 311, 326, 339,
353
- ScO 391
- self-consistent-field approximation, SCF
312
- SH 414
- SH⁺ 348
- SH⁻ 414
- Si₂C 364
- SiH 205, 282, 287, 413
- SiH⁺ 205
- Si(H₂)Si 423
- SiH₄ 105
- Silane plasma 413
- silicon compound 417
- SiN, dissociation energy 261
- SiO 44, 84, 105, 171, 282, 287, 317
- Slater determinant 311, 341
- smoothing 268, 269
- SnH 387
- SO, dissociation energy 263
- SO₂, dissociation energy 263
- solar continuum flux 231
- solar convection 201
- solar spectrum 197
- source function 57, 235, 238, 265
- spectrometer 296
- spectroscopic constants 312
- spectroscopy, infrared 18, 91, 98, 134,
412
- spectroscopy, intracavity loss absorp-
tion 370
- spectroscopy, long-path 367

- spectroscopy, millimeter wave 417
 spectroscopy, photoacoustic 369
 spectroscopy, ring-down cavity 371
 spectroscopy, time-resolved 383
 spectrum synthesis 287
 spectrum, rotational 417
 s-process elements 3, 13, 33, 44
 spin-orbit splitting 336
 SrO 389
 S stars 2, 33, 44, 126, 165, 319
 star formation 190
 stars, AGB 2, 113, 134
 stars, CH-type 67
 stars, M dwarfs 49, 61, 62, 92, 302
 stars, M sub dwarfs 61, 62
 stars, M-type 2, 33, 37, 49, 98, 165, 177, 296
 stars, Mira variables 59
 stars, S-type 2, 33, 44, 126, 165
 stars, barium 15, 18
 stars, brown dwarfs 61, 65, 91
 stars, carbon dwarfs 61, 67
 stars, carbon 6, 20, 33, 40, 69, 98, 101, 113, 134, 165, 177
 stars, dM 37
 stars, dwarfs 61
 stars, population III 215
 stars, population II 61
 stars, post-AGB 134
 stars, white dwarfs 61, 69, 72
 stellar atmosphere 30
 stellar atmosphere; see also model atmospheres
 stellar evolution 30, 71
 stellar nucleosynthesis 2
 stellar photosphere 30
 stellar spectra 303
 stellar structure 268
 stellar wind 130, 169
 stoichiometric compositions 180
 straight mean absorption coefficient 83
 strength, line 360
 strong line parameter 83
 supernova 2, 164
 symmetry, *e/f*-type 272
 SYNTHESIS 287
 temperature ambiguities 58
 thermodynamic equilibrium, TE 234
 TiH 387
 TiO 12, 37, 63, 244, 282, 287, 322, 391
 TiO₂ 39
 TiS 11
 transition dipole moment 228, 378
 transition energies 321
 transition moment function 314
 transition moment 274, 345, 377
 transition probability 59, 203, 274, 312, 316, 377
 transition, bound-bound 267
 transition, bound-free 267
 transition, electronic 197, 239
 transition, free-free 267
 transition, rotational 239
 transition, rotation-vibration 102
 transition, vibrational 239
 triatomic molecules 296
 variational technique 298
 vibronic coupling 330, 334
 vibronic functions 330
 VO 44, 59, 65, 287, 410
 Voigt analogue Elsasser band model, VAEBM 81, 88
 wavefunction, MORBID 359
 wavefunction, rovibrational 298, 354
 wavefunction, separation of 275
 wavefunction, vibrational 277, 329
 wavelength standards 400
 weak lines 9, 83, 279, 367
 white dwarf classes 73
 white dwarf cooling 72
 white dwarfs 61, 72, 215
 White cell 367
 YO 44, 391
 Zeeman effect 272
 ZnH 388
 ZrO 3, 16, 44, 287, 319, 391, 411
 ZrS 11