

Index

a

absorption cross sections 36–39
 – laboratory measurements
 – – CH₃OH 240
 – – H₂O 238
 – theoretical calculations
 – – Born-Oppenheimer approximation 235
 – – electronic potential energy surfaces 236–237
 – – oscillator strengths and cross sections 237–238
 acetamide 95
 acetic acid 95
 acetone, *see* propanone
 acetyl cyanide 95
 acid cyanides 95
 acidamides 95
 alkanolic acid 95
 alkanols, *see alkyl alcohols*
 alkyl alcohols
 – alkanediols and -polyols 82–83
 – butanol 82
 – methanol 77–79
 – propanol 81–82
 alkyl aldehyde 94–95
 alkyl cyanides
 – butyl cyanide 90–91
 – ethyl cyanide 89–90
 – methyl cyanide 89
 – propyl cyanide 90
 alkyl-substituted PAHs 67
 aluminium monoacetylde 25
 aminoacetonitrile 95
 aminoacids 95
 aminopropionitrile 96
 amorphous solid water (ASW)

– *c*-ASW, *see compact amorphous solid water (c-ASW)*
 – *p*-ASW, *see porous amorphous solid water (p-ASW)*
 Arrhenius-Kooij formula 114, 121
 ASW, *see amorphous solid water (ASW)*
 asymptotic giant branch (AGB)-stars 422–425, 428–430, 438–440, 442, 467, 472, 473, 478
 – PAHs 443–445
 Atacama large millimeter array (ALMA) 7, 75
 atom bombardment 292
 atomic force microscopy (AFM) 259
 aziridine 97

b

backscattering 126
 Born-Oppenheimer approximation 235
 broadband UV CO ice photodesorption 282, 293, 303, 310
 butanal 82, 95
 butanone 95
 butyl cyanide 90

c

carbon stars
 – AGB 438–440
 – equilibrium calculations 441–442
 – mineral formation 445
 – PAHs 443–445
 – WC-stars 440
 carbonaceous grains
 – condensation pathways 467–469
 – mid-IR spectrum 475–477
 – PAHs 471–473
 – soot formation 467
 – UV/vis spectral properties 474–475

- cationic PAHs 54–58
 - cavity ring-down spectroscopy (CRDS) 18, 30, 33–34
 - CFA, see *condensation flow apparatus (CFA)*
 - chemical master equation 313
 - chemical networks
 - carbonaceous species 111
 - chemical processes 111
 - dissociative recombination 116
 - gas phase processes 111
 - ion–molecule reactions 111
 - neutral–neutral reactions 116
 - radiative association 115–116
 - rate coefficients, temperature dependence of 114–115
 - rate equation 109
 - water formation 113
 - CO isotopolog photodissociation
 - ^{12}CO 248
 - Berkeley synchrotron source 248
 - interstellar radiation field 248
 - combustion process 451
 - compact amorphous solid water (c-ASW) 274, 276, 278–280, 282, 285
 - complex molecular spectroscopy
 - acid cyanides 95
 - acidamides 95
 - alkanolic acid 95
 - alkyl alcohols
 - – alkanediols and -polyols 82–83
 - – butanol 82
 - – ethanol 79–81
 - – methanol 77–79
 - – propanol 81–82
 - alkyl aldehyde 94–95
 - alkyl cyanides
 - – butyl cyanide 90
 - – ethyl cyanide 89–90
 - – methyl cyanide 89
 - – propyl cyanide 90
 - aminoacetonitrile 96
 - aminoacids 95
 - aminopropionitrile 96
 - aziridine 97
 - esters
 - – ethyl acetate 88
 - – ethyl formate 88
 - – methyl acetate 88
 - – methyl formate 87–88
 - ethanimine 96
 - ethers
 - – diethyl ether 86–87
 - – dimethyl ether 84–86
 - – ethyl methyl ether 86
 - ethylamine 94
 - galactic center sources 75
 - general spectroscopic considerations
 - – broad band sources 72
 - – large amplitude torsional motion 71
 - – rotational energy 69
 - – transition frequencies 71
 - glycine 72–73
 - glycolaldehyde 96
 - ketene 97
 - ketones 95
 - local thermal equilibrium (LTE) 72, 73, 75
 - mercaptans 91
 - methanimine 96
 - methylamine 91
 - moments of inertia 73
 - non-overlapping spectral features 73, 75
 - radio-astronomical detection 69
 - vinyl alcohol 96
 - vinyl cyanide 96
 - condensation Flow Apparatus (CFA) 456, 458, 459, 463, 466
 - configuration interaction (CI) method 236–237
 - corannulene 45
 - coronene 45
 - cosmic dust particles
 - AGB stars 332
 - diffuse interstellar medium 327, 329–330
 - infrared spectral region 329
 - molecular clouds 330–331
 - ultraviolet-visible wavelengths 327
 - cosmic standard mixture 420–422, 425, 430
 - cosmic-ray induced photons 244
 - CRDS, see *cavity ring-down spectroscopy (CRDS)*
 - crossed beam experiments
 - inelastic collisions 127
 - ion–molecule collisions 128
 - neutral–neutral collisions 124
 - radical–radical collisions 127
 - crystalline silicates 11
 - cyanomethanimine 96
 - cyanopolynes 4
- d**
- diffuse interstellar bands (DIBs) 3
 - degenerate four-wave mixing (DFWM) 18
 - dehydrogenated PAHs 66
 - deuterated PAHs 68
 - dibenzorubicene 46

- DIBs, see *diffuse interstellar bands (DIBs)*
- diethyl ether 86–87
- diffuse interstellar bands (DIBs) 15, 29
- anions 21
 - bare carbon chains 22–24
 - cations 20
 - CRDS 18
 - four-wave mixing technique 18
 - LIF 18–19
 - molecular ions 19
 - resonant two-color photodetachment 17
 - resonant two-color, two-photon fragmentation 17
 - resonant two-color, two-photon ionisation 17
- dimethyl ether 84–86
- direct master equation approach 314, 315
- direct photodissociation 230, 232
- dissociative recombination (DR) 116
- merged beam experiments 132
- dissociative UV ice photodesorption 305–306
- dust attenuation 245–246
- dust formation
- carbon stars 445
 - – AGB 438–440
 - – equilibrium calculations 441–442
 - – outflowing gas, molecular composition of 442–443
 - – PAHs 443–445
 - – WC-stars 440
 - condensation temperature 433–435
 - element abundances
 - – asymptotic giant branch (AGB) 422–423
 - – condensed phases, chemical equilibrium conditions 427–431
 - – cosmic standard mixture 420–422
 - – massive stars 425–426
 - – red giant branch (RGB) 422
 - first surface creation 431–433
 - hydrogenated carbon materials
 - – H atom irradiation 490–493
 - – ion bombardment 488–489
 - – thermal annealing 485–486
 - – UV irradiation 486–488
 - M-stars
 - – gas-phase composition 436
 - – seed particles 436–438
 - radiative transfer 419
 - reaction kinetics 435–436
 - silicate processing
 - – ion bombardment 480–483
 - – thermal annealing 478–480
 - – surface growth 433
- e**
- EDX, see *energy-dispersive X-ray (EDX) analysis*
- electron energy loss (EEL) spectrometer 452, 475
- Eley-Rideal abstraction mechanism 259, 265, 266, 268, 272, 312, 317
- energy-dispersive X-ray (EDX) analysis 452
- esters
- ethyl acetate 88
 - ethyl formate 88
 - methyl acetate 88
 - methyl formate 87–88
- ethane-1,2-diol 82–83
- ethanimine 96
- ethanol 79–81
- ethers
- diethyl ether 86–87
 - dimethyl ether 84–86
 - ethyl methyl ether 86
- ethyl acetate 88
- ethyl cyanide 89
- ethyl formate 88
- ethyl mercaptan 91
- ethyl methyl ether 86
- ethylamine 94
- Extended X-ray absorption near edge fine structure (EXAFS) 453, 475
- f**
- far-infrared spectroscopy (FIR) PAHs, 60–62
- FIR 60
- formamide 95
- formic acid 95
- formyl cyanide 95
- forsterite 7
- forward scattering 126
- four-wave mixing technique (FWM) 18
- g**
- gas-phase condensation particles, see *laboratory gas-phase condensation particles*
- gas-phase reactions 110
- glasses with embedded metals and sulfides (GEMS) particles 329
- glycerol 83
- glycine 95, 72–73
- glycolaldehyde 96
- guided ion beam (GIB) technique 130

h

- H₂O 242
- Herschel satellite
 - forsterite 7
 - photodesorption 5–6
 - TW Hya 6–7
 - water, distribution and abundance of 4
- hexabenzocoronene 46
- high-resolution transmission electron microscopy (HRTEM) 452, 457, 468
- hot atom reactions 259, 265, 266, 272
- HRTEM, see *high-resolution transmission electron microscope (HRTEM)*
- hydrogenated carbon materials
 - H atom irradiation 490–493
 - ion bombardment 488–489
 - thermal annealing 485–486
 - UV irradiation 486–488
- hydrogenated PAHs 66

i

- indirect photodissociation 237
- inelastic scattering
 - crossed beam experiments 127
 - density-to-flux conversion 170
 - initial state distribution 168
 - molecular beams
 - – crossed-beam scattering 165
 - – Newton spheres 165
 - – state-selective photoionization 166
 - predissociation model 169
 - relative collision cross sections 170
 - rotational energy level structure, water molecules 164–165
 - state-to-state cross section 163
 - temperature control 170
 - velocity map imaging technique 163
 - water–hydrogen molecule PES
 - – differential cross sections 174–175
 - – total cross sections 174
- infrared emission (IRE) spectroscopy 58
- infrared multiple photon dissociation (IRMPD) spectroscopy 57, 59, 65–67
- infrared Space Observatory (ISO) 330
- interplanetary dust particles (IDPs) 455
- interstellar dust grains
 - chemical structure 257
 - composition and size distribution 257
 - morphology 257
- interstellar grain size distribution 2–3
- interstellar molecular ions 1
- interstellar radiation field (ISRF) 242–243, 247, 248, 299
- interstellar surface astrochemistry

- astrochemical network models
 - – kinetic Monte Carlo approach 316–318
 - – modified rate equations 316
 - – rate equations 310–313
 - – stochastic methods 313–316
 - chemical complexity in space
 - – H-atom bombardment, see *atom bombardment*
 - – vacuum UV irradiation, see *UV ice photodesorption*
 - ice morphology
 - – ASW 273–276
 - – carbon monoxide (CO) 282–287
 - – H₂ reaction, energetic balance of 281–282
 - – hydrogen sticking 278–279
 - – ion and UV photon irradiation 287–289
 - – molecular hydrogen desorption 276–278
 - – recombination process 279–281
 - molecular hydrogen (H₂) formation
 - – carbonaceous surfaces 264–269
 - – energy partitioning 269–272
 - – physisorbed and chemisorbed hydrogen atoms 263
 - off-surface methods 260
 - on-surface methods
 - – global techniques 260
 - – local techniques 259
 - intramolecular vibrational redistribution (IVR) 57
 - ion–molecule collisions 128
 - ion Neutral Mass Spectrometer (INMS) 162
 - ion–molecule reactions 111
 - IRMPD, see *infrared multiple photon dissociation (IRMPD) spectroscopy*
- k**
- ketene 97
 - ketenimine 97
 - kinetic Monte Carlo approach 316–318
- l**
- laboratory gas-phase condensation particles
 - analytical tools
 - – EDX analysis EDX 452–453
 - – electron energy loss (EEL) spectrometer 452
 - – HRTEM 452
 - – MALDI-TOF analysis 454
 - – spectroscopic and chromatographic methods 453–454

- X-ray absorption and scattering spectroscopy 453
- carbonaceous grains
- condensation pathways 467–469
- mid-IR spectrum 475–477
- PAHs 471–473
- soot formation 467
- UV/vis spectral properties 474–475
- combustion process 451
- LIP 450–451
- magnesium iron silicates
- CFA 456–458
- deep metastable eutectic (DME) composition 460
- equilibrium condensation 455
- grain types 458
- HRTEM analyses 457
- solar nebula 455
- thermal annealing 464–466
- plasma based nucleation 451
- production steps 448
- pulsed laser ablation 448–449
- laboratory IR spectroscopy, PAHs
- alkyl-substituted PAHs 67
- cationic PAHs 54–58
- CC-stretching modes 65
- computational methods 58
- deuterated PAHs 68
- FIR 60–61
- five-membered rings 68
- hydrogenated and dehydrogenated PAHs 66
- metal PAH complexes 67
- neutral PAHs 53–54
- nitrogen substituted PAHs 65
- protonated PAHs 65
- vibrational mode characters 63–64
- Langmuir-Hinshelwood diffusive mechanism 258, 265, 268, 271, 272, 295, 312, 313, 317
- laser induced thermal desorption time-of-flight (LITD-TOF) 260
- laser-induced fluorescence (LIF) 18–19, 30
- laser-induced pyrolysis (LIP) 450–451, 468, 476
- LIF, see *laser-induced fluorescence (LIF)*
- linear polyacetylene cations 20
- LIP, see *laser-induced pyrolysis (LIP)*
- low temperature collisions 132–134
- luminous blue variables (LBV) 426, 428
- Lyman α radiation 244
- m**
- M-stars
- gas-phase composition 436
- seed particles 436–438
- macroscopic stochastic methods 313
- magnesium iron silicates condensation
- CFA 456–458
- deep metastable eutectic (DME) composition 460
- grain types 458
- HRTEM analyses 457
- solar nebula 455
- thermal annealing 464–466
- mass-analyzed threshold ionization (MATI) spectra 62
- massive stars 425–426
- matrix isolation spectroscopy (MIS) 30, 35–37, 39, 45, 53, 56, 57, 59, 66
- merged beam experiments
- dissociative recombination 132
- guided ion beam (GIB) technique 130
- integral cross section 128
- low collision energies 128
- radiative detachment 132
- single collision conditions 131
- metal PAH complexes 67
- metallicity 420, 422, 424, 426, 439
- methanal 94
- methanediol 82
- methanimine 96
- methanol 77–79
- methyl acetate 88
- methyl cyanide 89–90
- methyl formate 87–88
- methyl mercaptan 91
- methylamine 91
- methylated PAHs 67
- MgCN 24
- MgS 438, 446
- microscopic stochastic methods 313
- MIS, see *matrix isolation spectroscopy (MIS)*
- molecular hydrogen formation 8
- molecular photodissociation, see *photodissociation*
- molecular spectroscopy
- complex molecules, see *complex molecular spectroscopy*
- DIBs
- anions 21
- bare carbon chains 22–24
- cations 20
- CRDS 18
- four-wave mixing technique 18
- LIF 18–19
- molecular ions 19
- resonant two-color photodetachment

- molecular spectroscopy (*contd.*)
 - – resonant two-color, two-photon fragmentation 17
 - – resonant two-color, two-photon ionisation 17
 - PAHs
 - – laboratory IR spectroscopy, see *laboratory IR spectroscopy, PAHs*
 - – UV/vis gas phase absorption spectroscopy, see *UV/vis gas phase absorption spectroscopy, PAHs*
- multiplex integrated cavity output spectroscopy (MICOS) technique 34
- n**
- Nebulium lines 1
- neutral–neutral collisions 124
- neutral PAHs 53–54
- neutral–neutral reactions 116
- Newton spheres 163, 165
- nitrogen substituted PAHs 65
- non-dissociative UV ice photodesorption 303–304
- o**
- Ostwald ripening 458
- oxides 11
- p**
- PDR, see *photon-dominated region (PDR)*
- perylene 37, 38, 41, 42, 45
- photo dissociation regions (PDRs) 258, 259, 262, 268, 269, 272
- photodesorption 5–6
- photodissociation
 - CO
 - – ^{12}CO 248
 - – Berkeley synchrotron source 248
 - – cosmic-ray induced photons 244
 - – cross sections 238 see also *absorption cross sections*,
 - definition 229
 - diatomic molecules
 - – direct photodissociation 230
 - – OH radical 232
 - – predissociation 230
 - – spontaneous radiative dissociation 231
 - dust attenuation 245–246
 - ISRF 242–243
 - large molecules
 - – internal conversion 233
 - – intersystem crossing 233
 - – ionization potentials 234
 - Lyman α radiation 244
 - N_2 249
 - PAHs
 - – H-loss channel, small molecule 250
 - – large molecule 249
 - – PIRENEA 250
 - product branching ratios 240, 241
 - rate of
 - – continuous absorption 246–247
 - – depending factors 229
 - self-shielding 246
 - small molecules 230–233
 - stellar radiation fields 243
 - photodissociation rates 10
 - photon-dominated region (PDR) 4, 10, 229
 - PIRENEA experiment 250
 - plasma based nucleation 451
 - polycyclic aromatic hydrocarbons (PAHs) 3, 10, 269, 467, 470
 - H-loss channel, small molecule stability 250
 - laboratory IR spectroscopy
 - – alkyl-substituted PAHs 67
 - – cationic PAHs 54–58
 - – CC-stretching modes 65
 - – computational methods 58
 - – deuterated PAHs 68
 - – FIR 60–61
 - – five-membered rings 68
 - – hydrogenated and dehydrogenated PAHs 66
 - – metal PAH complexes 67
 - – mid-infrared spectra 49, 50, 54
 - – neutral PAHs 53–54
 - – nitrogen substituted PAHs 65
 - – protonated PAHs 65
 - – vibrational mode characters 63–64
 - large molecule stability 249
 - PIRENEA 250
 - UV/vis gas phase absorption spectroscopy
 - – astronomical vs. laboratory-based spectra 31, 40–41
 - – corannulene 45
 - – coronene 45
 - – CRDS 30, 33–34
 - – dibenzorubicene 46
 - – DIBs 29
 - – dispersion interaction energy 39
 - – equivalent band width 42
 - – experimental uncertainty 42
 - – gas phase transitions, extrapolation of 39–40
 - – hexabenzocoronene 46
 - – laser-induced pyrolysis 47–48
 - – LIF 30

- – MIS 31, 35–36
- – oscillator strength 42
- – photoabsorption cross sections 36–39
- – size 30
- – supersonic jet technique 30
- polycyclic aromatic hydrocarbons (PAHs) 443–445, 471–473
- porous amorphous solid water (p-ASW) 274–276, 278–283
- potential energy surface (PES) 125, 126
- predissociation 230, 232
- propanal 94
- propanediol 83
- propanol 81–82
- propanone 95
- propionamide 95
- propionic acid 95
- propyl cyanide 90
- protonated PAHs 65
- protonated polyacetylenes 21
- pulsed laser ablation 448–449

r

- radiative association (RA) 115–116
- radiative attachment 135
- radiative detachment 132
- rainbow scattering 167
- red giant branch (RGB) 422, 425, 428
- reflection-absorption infrared spectra (RAIRS) 292, 294, 295, 301, 305, 308
- refractory elements 420, 425–427, 429, 430, 441
- resonance enhanced multiphoton ionization (REMPI) 164, 166, 240, 260
- resonant two-color photodetachment (R2CPD) 17
- resonant two-color, two-photon fragmentation (R2C2PF) 17
- resonant two-color, two-photon ionisation (R2C2PI) 17
- Rice-Ramsperger-Kassel-Marcus (RRKM) theory 234
- rock-forming elements 421

s

- scaled NEXTGEN model radiation field 244
- scanning tunneling microscopy (STM) 259
- scattering process
 - deflection function 117
 - diatomic collision 117
 - differential cross sections 119–120
 - integral cross section 119
 - ion induced dipole interaction 121
 - state specific rate coefficients 119

- selected ion flow tube (SIFT) 134–136
- self-shielding 246
- SiC 446
- SIFT, see *selected ion flow tube (SIFT)*
- silicate processing
 - ion bombardment 480–483
 - thermal annealing 478–480
- Spitzer spectroscopy 331
- spontaneous radiative dissociation 231, 232
- Stardust 332–334
- state-to-state differential cross sections (DCSs) 163
- stellar radiation fields 243
- supergiants 425, 428, 434
- supersonic jet technique 30
- SURFace Reaction Simulation Device (SURFRESIDE²) 294, 295, 301
- surface reactions, interstellar conditions
 - off-surface methods 259, 260
 - on-surface methods 259
 - water ice layers 257

t

- temperature programmed desorption (TPD) 260, 274, 277, 278, 280, 283–285, 291, 294, 301
- thermal rate coefficients 134
- TiC nanoparticles 445
- TW Hya 5, 6
- two-color resonant four-wave mixing (TC-RFWM) 18

u

- ultraviolet and visual echelle spectrograph (UVES) 41
- Ulysses and Galileo satellites 2
- unidentified infrared bands (UIRs) 52
- UV ice photodesorption
 - dissociative 305–306
 - efficiencies 306
 - non-dissociative 303–304
- UV/vis gas phase absorption spectroscopy, PAHs
 - astronomical vs. laboratory-based spectra 31, 40–41
 - corannulene 45
 - coronene 45
 - CRDS 30, 33–34
 - dibenzorubicene 46
 - DIBs 29
 - dispersion interaction energy 39
 - equivalent band width 42–43
 - experimental uncertainty 42

UV/vis gas phase absorption spectroscopy,

PAHs (*contd.*)

- gas phase transitions, extrapolation of 39–40
- hexabenzocoronene 46
- laser-induced pyrolysis 47–48
- LIF 30
- MIS 31, 35–36
- oscillator strength 42
- photoabsorption cross sections 36–39
- size 30
- supersonic jet technique 30

v

velocity map imaging (VMI) 163, 166, 240
vinyl alcohol 96
volatile elements 421

w

water abundance 4–5
water ice 330
WC-stars 426, 429, 440, 446
WN-stars 426, 446
Wolf-Rayet (WR) stars 422, 467

x

X-ray absorption near edge structure (XANES) 453

z

zero-kinetic energy photoelectron spectroscopy (ZEKE-PES) 62