

## Index

### **a**

- ALC- $\mu$ SR spectroscopy
  - for  $^{13}\text{C}$  hyperfine coupling constants in  $^{13}\text{C}_6\text{H}_6\text{Mu}$  37
  - for  $^1\text{H}$  hyperfine coupling constants in  $\text{C}_6\text{H}_6\text{Mu}$  37
  - in anisotropic environments 232–234
  - in isotropic environments 230–232
  - of  $^{13}\text{C}_{60}\text{Mu}$  radical in decalin solution 162, 163
  - of methylene proton  $\Delta_0$  resonance 129
  - of Mu adducts
    - of 5CB in nematic and isotropic phases 188
    - of MBBA in isotropic and nematic phases 184
    - of 2-phenylethanol in aqueous  $\text{NiCl}_2$  solutions 193
  - of muoniated cyclohexadienyl radical 37, 38
  - of muoniated radicals 34–39
  - of muoniated *tert*-butyl radical in NaY and USY zeolites 169, 171
  - of [2.2]-paracyclophane powder 39
  - of PEA in DHTAC 191, 192
  - of purine bases 207
  - of pyrimidine bases 209
  - of tris[8-hydroxyquinoline]aluminium ( $\text{Alq}_3$ ) 205, 206
- $\alpha$ -muoniated radicals 58

### **b**

- backward muon beams 12
- $\beta$ -muoniated radicals 58
- Bethe–Bloch stopping-power formula 46
- bilayers and micelles 190–195
- bimolecular reactions, rate calculations
  - for 71–73
- biological systems 207–212
- biomembranes 193–194
- 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-pentacene) 205
- Bloch equations 145
- Born–Oppenheimer Approximation 67, 68, 111
- Breit–Rabi diagram 24, 29
- Br–Mu–Br vibrational bonding 84–86

### **c**

- calamitic liquid crystals 182
- charge states of muons 1, 45–48
- chemical kinetics 65–67
  - in liquids vs. gases 89–90
  - pH dependence 99–101
  - pressure and density dependence 92–96
  - reaction vs. spin relaxation 82
- clathrates, muonium and muoniated radicals in 164–167
- $\text{C}_{60}\text{Mu}$  spin system, energy levels and transitions for 161

- Collisions per encounter 92–93, 95  
 Collision theory 71–72  
 conjugated polymers, electron conduction  
   in 199–202  
 continuous vs. pulsed muon beams  
   14–16  
 cosurfactants, in bilayers and micelles  
   190–195  
 C<sub>60</sub> and C<sub>70</sub> structures 163, 164  
 4-cyano-4'-pentylbiphenyl (5CB) 182  
   fluctuations of 187–190  
 cyclohexadienyl-type Mu adducts, of 5CB  
   187, 188  
 cytochrome C 210
- d**  
 defect diffusion model 200  
 DHTAC 191–192  
 diamagnetic muons  
   in longitudinal field 18–19, 223–224  
   in transverse field 19–22, 224–225  
   in zero magnetic field 22, 23  
 diamagnetic muon spin relaxation 143  
 diffusion-limited reactions 90  
 dipole–dipole reaction field model 129  
 DNA and its constituents 207–209  
 dynamic processes, in non-conjugated  
   polymers 195–199
- e**  
 electric field effects on Mu formation 53  
 electron conduction, in conjugated  
   polymers 199–202  
 electron spin-flip exchange cross section  
   149  
 electron vs. nuclear spin relaxation rates  
   147  
 Ergodic Principle 65, 78, 145  
 experimental muon techniques 4, 16–18
- f**  
 Fermi contact interaction 107, 120, 157  
 field modulation in ALC- $\mu$ SR 35  
 fluctuation-rate dependence, of zero-field  
   depolarization function 22, 23  
 forward muon beams 13  
 fullerenes, muonium and muoniated  
   radicals in 160–164
- g**  
 Gaussian Kubo–Toyabe relaxation  
   function 22  
 Gaussian relaxation 20–21
- h**  
 H abstraction, by muonium 54  
 H atom abstraction reactions 75–77  
 H + formic acid reaction 100  
 hot-atom reactions 6, 45, 49  
 hydrogen isotopes 2, 158
- i**  
 isolated resonance model (IRM) 84  
 isotropic environments  
   muoniated radicals in 227–228  
   muon spin resonance in 230–232  
 isotropic hyperfine coupling constants  
   of  $\alpha$  nuclei 108–110  
   of  $\beta$  nuclei 110–111
- k**  
 Karplus–Fraenkel equation 110, 162  
*keto-enol* tautomerism 57
- l**  
 LF- $\mu$ SR 18  
   of PANI:EB 202  
   of polystyrene 195, 196  
   of tris[8-hydroxyquinoline]aluminium  
     (Alq<sub>3</sub>) 204  
 Lindemann kinetics 80–81  
 liquid crystals  
   ESR studies 183  
   magnetic resonance techniques 182  
   thermotropic 181–190  
 localized defects, in organic  
   semiconductors 204–206  
 longitudinal field repolarization studies,  
   of muoniated radicals 40–43

longitudinal-field repolarization  
 technique 85  
 low-energy muon beams 13, 219

## **m**

magnetic ordering, in organic materials  
 202–203

matrix isolation strategy 217

MBBA 182

orientational ordering of 184–187

$\mu^-$  capture and muonic atoms 60–61

$\mu^+$  charge exchange, in gas phase 45–49

MELODY 219

$\mu$ SR spectrometers 16–18

Mu addition

to alkenes, dienes and allenes 54

to alkynes 56–57

to benzene and aromatic compounds  
 54–56

to carbenes and related

electron-deficient molecules 59

to carbonyls and thiocarbonyls 57–58

to diazo compounds 58–59

to heteroatom unsaturated bonds 238

to ketenes 58–59

Mu and H kinetics, in liquid phase  
 99–101

Mu formation

and track effects in dense media  
 49–53

in gas phase 45–49

Mu + halogens 73, 74

Mu + H<sub>2</sub>O<sub>2</sub> complex reaction system  
 102–104

Mu + OH<sup>-</sup> reaction 94

Muonation vs. muoniation 3

muon beams

backward 12

continuous vs. pulsed 14–16

surface 12

muon decay and detection 13–14

muon facilities 4, 14–16, 219

muon fractions 47–51

muoniated cyclohexadienyl radicals 54,  
 99, 108–110, 122, 174, 177, 185, 215

ALC- $\mu$ SR spectra 37, 38

in NaY zeolite 169

on silica powder surfaces 173

muoniated radicals 3

avoided level-crossing resonance of  
 34–39

characterization by muon spin  
 spectroscopy 136

radicals containing metal atom  
 138–139

radicals containing phosphorus  
 137–138

radicals containing Si or Ge  
 136–137

with no additional nuclear spins  
 139–140

formation by ionic mechanism 59

from proteins 209–212

in anisotropic environments 32,  
 227–228

in high transverse fields 228–229

in isotropic environments 28, 227–228

in longitudinal fields 229–230

intramolecular motion

methyl radicals 116–118

Mu adducts of carbonyls 119–120

other alkyl radicals 119

*tert*-butyl radical 116

in zeolites 167–172

isotope effects

bond length 111–113

conformational preference 114–116

hyperfine constants 113–114

isotropic hyperfine coupling 107–111

longitudinal field repolarization studies  
 of 40–43

methyl radical 32, 58, 59, 109

reorientational dynamics

anisotropic motion in solids 128

dipolar hyperfine coupling constants  
 120–123

effect of hyperfine anisotropy  
 124–128

RF muon spin resonance of 39–40

- muoniated radicals (*contd.*)
    - solvent effects on hyperfine coupling
      - constants 129–131
    - spin relaxation in 150–153
    - TF- $\mu$ SR 28–34
    - vinyl radicals 57
  - muonic helium atom 1–2, 75
  - Muon Induced X-Ray Emission (MIXE)
    - spectroscopy 219
  - muonium
    - chemistry, development of 5–7
    - decay kinetics 6, 65–67, 89–90
    - diffusion in water 90–92
    - in confined spaces 157–159
    - in longitudinal fields 26–28, 226–227
    - in transverse field 24–26, 225–226
    - spectroscopy 23–28
    - spin exchange, with paramagnetic species 147–150
  - muonium and muoniated radicals
    - in clathrates 164–167
    - in fullerenes 160–164
    - on surfaces 172–177
  - muonium- $C_{60}$  system 160
  - muon rest mass 1
  - muon spin flip 233
  - muon spin operator 224
  - muon spin polarization,
    - residual polarization 104
    - transfer from precursor to radical 33–34
    - transfer from primary to secondary radical 134–135
  - muon spin relaxation 143
    - aqueous solutions of Manganese(II) ions 145–147
    - due to spin exchange 147–150
    - during chemical reaction 153–155
    - molecular dynamics from 143–145
  - muon spin spectroscopy ( $\mu$ SR)
    - advantages 65, 216
    - limitations 216, 220
    - outlook 219–220
    - sensitivity of 4
    - spin manipulation 218
    - transient targets 217
      - with optical spectroscopy 217–218
  - muon thermalization 46–48, 67
  - muon tomography 218–219
  - MuSIC 219
- n**
- $^{23}\text{Na}$  hyperfine coupling constants 171
  - negative muon thermalization 61
  - N*-(4-methoxybenzylidene)-4-butylaniline (MBBA) 182
    - orientational ordering of 184–187
  - N*-muono-pyridinyl radical 110
  - non-conjugated polymers, dynamic processes in 195–199
  - Noyes equation 90
- o**
- operando experiment 217
  - organic materials, magnetic ordering in 202–203
  - organic semiconductors, localized defects in 204–206
- p**
- PEA (2-phenylethanol) 191–194
  - pH dependence 99–101, 102–104
  - p*-nitrophenyl nitronyl nitroxide (p-NPNN) 202, 203
  - polarons 199, 200
  - polyaniline:emeraldine base (PANI:EB) 201, 202
  - polymers
    - dynamic processes in non-conjugated polymers 195–199
    - electron conduction in conjugated polymers 199–202
  - potential energy surface (PES) 67–71
    - contour plot in isoenergetic coordinates 69
    - for Br–H–Br 86
    - for collinear H atom exchange reaction 68
    - for H–Br–Br 85
  - proteins, muoniated radicals formed from 209–212

proton beams, time structures of 15  
 pulsed muon sources, advantage of 16  
 pulse radiolysis studies 95, 96, 103  
 pyrazine 101, 102

**q**

quantum mass effects  
   in kinetics 67–71  
   in vibrational bonding 84–86  
 quantum mechanical trajectory (QMT)  
   calculation 72  
 quasiclassical trajectories (QCT) 72

**r**

rate constants  
   for Mu/H addition to alkenes 236  
   for Mu/H addition to aromatic  
     compounds 237  
   for Mu/H addition to heteroatom  
     unsaturated bonds 238  
   for Mu with methanol 96  
   for Mu with oxalic acid 101  
   for Mu with the formate anion 100  
 Redfield formalism 174  
 reduced hyperfine constant 107  
 repolarization technique 27, 28  
 residual polarization analysis 104  
 restricted-random-walk model, of  
   orientational ordering 186, 187  
 RF muon spin resonance, of muoniated  
   radicals 39–40  
 Risch–Kehr (RK) model 201  
 rotational potential, for CH<sub>2</sub>Mu group  
   115

**s**

silsesquioxanes 157, 158, 160  
 single-component phase diagram 93  
 singly-occupied molecular orbital  
   (SOMO) 107, 109–111, 115–117,  
   119, 121, 122, 204  
 Smoluchowski equation 90  
 soft matter 181  
 solitons 200  
 solvent effects on hyperfine coupling  
   constants 129–131

spin density 107–110,  
   in C<sub>60</sub>Mu and C<sub>70</sub>Mu 163, 164  
   in methyl radical 117  
 spin-exchange reactions 94, 147–150  
 spin-lattice relaxation time 144  
 spin-polarized muon beams 11–13  
 spin probes 183  
 spin relaxation  
   in muoniated radicals 150–153  
   molecular dynamics from 143–145  
 spur model of muonium formation 6,  
   50–53, 217  
 state-selected reactivity 77–79  
 stochastic Liouville approach 175  
 Stokes–Einstein equation 90  
 surface muon beams 12, 73  
 surfactant-based bilayers 193  
 surfactants 190

**t**

TF-μSR spectra  
   of C<sub>60</sub> 160  
   of C<sub>6</sub>H<sub>6</sub>Mu and C<sub>6</sub>D<sub>6</sub>Mu 30  
   of muoniated radical on silica grains  
     173  
     in anisotropic environments 32–33  
     in isotropic environments 28–32  
 thermotropic liquid crystals 181–190  
 transition state theory (TST) 72, 73

**v**

van der Waals complex 84–86  
 velocity scaling 46  
 vibrational adiabaticity 70  
 vibrational bonding 84–86

**z**

zeolites, muoniated radicals in 167–172  
 zero-field muon spin relaxation (ZF-μSR)  
   spectra  
   of p-NPNN 203  
   of polyethylene 22, 23  
 zero-point energy (ZPE) 68, 70, 72, 75,  
   86, 91, 112, 114  
 zero-point vibrational isotope effects  
   112, 113

