

Index

a

- acetylene complexes 109–111
- acquisition time 8
- agostic interaction 226
- allyl and Cp anions 79–83
- allyl and Cp complexes
- ^{13}C chemical shifts for 111–119

b

- beta-hydrogen elimination 315
- bidentate 329, 358
- bidentate olefin ligands 76
- bisphosphine complexes, ^{13}C spectra of
 - second-order effects in 251–254
- σ -bound alkyl groups 73, 74
- σ -bound alkyl, aryl, and alkynyl complexes 89–99
- σ -bound carbon 365, 366, 368
- π -bound olefin complexes 99–108

c

- carbenes 125–130, 131, 327, 343, 351, 358, 359
- carbene ligands 83–84, 85
- carbonyl complexes, ^{13}C chemical shifts in 119–125
- carbynes 125–130, 131
- $\eta^3\text{-C}_3\text{H}_5$ complexes, ^{13}C data for 114
- ^{13}C chemical shift 87
 - acetylene complexes 109–111
 - allyl and Cp complexes 111–119
 - carbenes, carbynes, and related complexes 125–130
 - carbonyl complexes 119–125
 - N-heterocyclic carbenes 130–133
 - π -bound olefin complexes 99–108
 - σ -bound alkyl, aryl, and alkynyl complexes 89–99

^{113}Cd chemical shifts 186

- chemical shift anisotropy 15–16
- chemical shifts 63
 - ^{13}C 87
- acetylene complexes 109–111
- allyl and Cp complexes 111–119
- carbenes, carbynes, and related complexes 125–130
- carbonyl complexes 119–125
- N-heterocyclic carbenes 130–133
- π -bound olefin complexes 99–108
- σ -bound alkyl, aryl, and alkynyl complexes 89–99
- ^{19}F NMR 147–155
- ^1H NMR
- allyl and Cp anions 79–83
- anisotropic effects 64–67
- carbene ligands 83–84, 85
- hydrides 67–71
- molecular H_2 and $\eta^2\text{-X-H-M}$ complexes with X = C, Si, and H 72–73
- η^2 , η^4 -Olefin, and η^6 -arene proton chemical shifts 74–79
- σ -bound alkyl groups 73, 74
- heavy atom NMR 84, 86
- ^{15}N NMR 134–146
- ^{31}P NMR 155–179
- transition metals 180–197
- ^{59}Co and ^{103}Rh , oxidation state and chemical shift for 186
- CO ligands, bonding modes for 120
- ^{13}CO NMR 119–125
- COSY spectrum 20
- coupling constants 207
 - $^1J(\text{C},\text{H})$ in $\eta^2\text{-C-H}\cdots\text{M}$ complexes 222–225
 - $^1J(\text{H},\text{D})$ and molecular hydrogen complexes 220–222

- c**
- coupling constants (*contd.*)
 - $^1J(\text{Si},\text{H})$ in $\eta^2\text{-Si-H}\cdots\text{M}$ complexes 226–230
 - 1J , applications involving 219–220
 - background 207–208
 - one-bond interactions 208–216
 - remote agostic bonds 226
 - trans influence and 1J 230–238
 - two- and three-bond J -values 238
 - geometric dependence of $^2J(\text{L}^1\text{-M-L}^2)$ 254–255
 - $^2J(^{31}\text{P},^{13}\text{C})$ 264–265, 265
 - $^2J(^{31}\text{P},^{19}\text{F})$ 266–272
 - $^2J(^{31}\text{P},^{31}\text{P})$ 258–264, 271
 - $^2J(^{31}\text{P-M-}^1\text{H})$ 255–256
 - $^2J(\text{X},^1\text{H})$ 256–258
 - ^{31}P and ^{13}C J -values 249–251
 - routine ^1H coupling constants 242–246
 - second-order effects in ^{13}C spectra of bisphosphine complexes 251–254
 - two and three-bond ^{31}P coupling constants with ^1H 246–248
 - 1,5-cyclooctadiene (1,5-COD) 77, 105, 193
 - 2-D NOESY 43–49
- d**
- density functional theory (DFT) 68
 - diffusion constants, via NMR measurements, 55–60
 - dinuclear hafnocene 1,3-butadiyne salt 111
 - 1,3-diphenyl allyl Pd salts 115
 - dipole–dipole relaxation 12–14, 39, 42, 44
 - DOSY 55, 57, 58, 60
 - dwell time (DT) 8–9
 - dynamics 279–280
 - line shape analysis 284–290
 - magnetization transfer 291–296
 - two-dimensional NMR and chemical exchange 296–308
 - variable temperature 280–284
- e**
- exchange spectra 298, 300, 304–305, 308
- f**
- Fe(Cp) salt 228
 - Fe(diene)L3-complexes, $\delta^{31}\text{P}$ NMR data for 175
 - ^{19}F excursion 216–219
 - ^{19}F NMR 147–155
 - free induction decay (FID) 7, 8
- h**
- β -H elimination 364, 366
 - heavy atom NMR 84, 86
 - HMQC and HMBC 21
 - methods 21–22
 - one-bond 2-D $^{13}\text{C},^1\text{H}$ correlations 22–25
 - one-bond 2-D $^{15}\text{N},^1\text{H}$ correlations 25–26
 - two and three long-range bond $^{13}\text{C},^1\text{H}$ correlations 26–31
 - $\text{X},^1\text{H}$ correlations 31–36
 - HOESY 50–51
 - ^1H NMR
 - η^2 , η^4 -olefin, and η^6 -arene proton chemical shifts 74–79
 - σ -bound alkyl groups 73, 74
 - allyl and Cp anions 79–83
 - anisotropic effects 64–67
 - carbene ligands 83–84, 85
 - hydrides 67–71
 - measurement 7
 - molecular H_2 and $\eta^2\text{-X-H-M}$ complexes with $\text{X} = \text{C, Si, and H}$ 72–73
 - hydride 67–71, 361, 362, 363, 364, 377, 378, 379, 385
 - hydrodynamic radius 57, 58
- i**
- interligand NOEs 40, 45
 - ion pairing 59–60
 - isomer 319, 320, 323, 330, 331, 337–338, 352
 - 1J , applications involving 219–220
 - $^{2,3}J(^1\text{H},^1\text{H})$ 242
 - $^{1}J(^1\text{H},^2\text{H})$ 221–222, 221
 - $^{3}J(^1\text{H},^1\text{H})$ 243, 244
 - $^{1}J(^{13}\text{C},^1\text{H})$ 212, 215, 222–223, 224, 225
 - $^{2}J(^{13}\text{C},^1\text{H})$ 26
 - $^{3}J(^{13}\text{C},^1\text{H})$ 26
 - $^{1}J(^{29}\text{Si},^1\text{H})$ 209, 227
 - $^{2}J(^{29}\text{Si},^1\text{H})$ 33–34
 - $^{1}J(^{31}\text{P},^1\text{H})$ 208
 - $^{2}J(^{31}\text{P},^1\text{H})$ 246
 - $^{3}J(^{31}\text{P},^1\text{H})$ 246, 247
 - $^{1}J(^{31}\text{P},^{13}\text{C})$ 249–250, 249
 - $^{1}J(^{31}\text{P},^{19}\text{F})$ 217, 218
 - $^{2}J(^{31}\text{P},^{13}\text{CO})$ 239
 - $^{2}J(^{31}\text{P},^{31}\text{P})$ 242, 264–265, 265
 - $^{2}J(^{31}\text{P},^{19}\text{F})$ 266
 - $^{2}J(\text{X},^{31}\text{P})$ 267–272
 - $^{2}J(^{31}\text{P},^{31}\text{P})$ 258–264, 271
 - $^{3}J(^{31}\text{P},^{13}\text{C})$ 246
 - $^{n}J(^{31}\text{P},^{13}\text{C})$ 250
 - $^{2}J(^{31}\text{P-M-}^1\text{H})$ 255–256
 - $^{2}J(^{31}\text{P-M-}^{13}\text{C})$ 254
 - $^{2}J(^{31}\text{P-M-}^{31}\text{P})$ 254

- J***
- $^1J(^{103}\text{Rh}, ^{19}\text{F})$ 218
 - $^1J(^{103}\text{Rh}, ^{31}\text{P})$ 212, 214, 218, 230
 - $^2J(^{107,109}\text{Ag}, ^{19}\text{F})$ 212
 - $^1J(^{109}\text{Ag}, ^{31}\text{P})$ 211
 - $^1J(^{183}\text{W}, ^{31}\text{P})$ 215, 270
 - $^1J(^{195}\text{Pt}, ^{111,113}\text{Cd})$ 210
 - $^1J(^{195}\text{Pt}, ^{13}\text{C})$ 212, 231, 232, 232
 - $^3J(^{195}\text{Pt}, ^{13}\text{C})$ 243
 - $^1J(^{195}\text{Pt}, ^{13}\text{CO})$ 232
 - $^1J(^{195}\text{Pt}, ^{15}\text{N})$ 237, 238
 - $^1J(^{195}\text{Pt}, ^{195}\text{Pt})$ 210
 - $^1J(^{195}\text{Pt}, ^{19}\text{F})$ 219
 - $^1J(^{195}\text{Pt}, ^1\text{H})$ 209, 226
 - $^1J(^{195}\text{Pt}, ^{31}\text{P})$ 215, 233, 234, 235, 236
 - $^1J(^{19}\text{F}, ^1\text{H})$ 218–219
 - $^1J(\text{C}, \text{H})$ in $\eta^2\text{-C-H} \cdots \text{M}$ complexes 222–225
 - $^1J(\text{H}, \text{D})$ and molecular hydrogen complexes 220–222
 - $^2J(\text{L}^1\text{-M-L}^2)$, geometric dependence of 254–255
 - $^1J(\text{Si}, \text{H})$ in $\eta^2\text{-Si-H} \cdots \text{M}$ complexes 226–230
 - $^2J(\text{X}, ^1\text{H})$ 256–258
 - J -values, two- and three-bond 238
 - geometric dependence of $^2J(\text{L}^1\text{-M-L}^2)$ 254–255
 - $^2J(^{31}\text{P}, ^{13}\text{C})$ 264–265, 265
 - $^2J(^{31}\text{P}, ^{19}\text{F})$ 266
 - – $^2J(\text{X}, ^{31}\text{P})$ 267–272
 - $^2J(^{31}\text{P}, ^{31}\text{P})$ 258–264, 271
 - $^2J(^{31}\text{P-M-}^1\text{H})$ 255–256
 - $^2J(\text{X}, ^1\text{H})$ 256–258
 - ^{31}P and ^{13}C J -values 249–251
 - routine ^1H coupling constants 242–246
 - second-order effects in ^{13}C spectra of bisphosphine complexes 251–254
 - two and three-bond ^{31}P coupling constants with ^1H 246–248
- k***
- Karplus-type relation 242
- l***
- line shape analysis 284–290
- m***
- magnetization transfer 291–296
 - metal alkyl complexes 73
 - Mo complexes, ^{31}P NMR data for 176
- n***
- N-heterocyclic carbenes (NHCs) 127, 130–133
 - NMR-active transition metals 182
 - NMR problems 323–360
- p***
- ^{31}P and ^{13}C J -values 249–251
 - P(aryl)₃ complexes 13
 - Pd(0) divinyl silane phosphine complexes, ^{31}P Data for 166
 - Pd(η^3 -1,3-diphenylallyl)(chelate) cations 133
 - PdH(SiH(*t*-Bu)₂)₂(1,2-bis(dicyclohexylphosphino)ethane) 255
 - Pd-CH₃ ^{13}C chemical shift 91
 - phase-sensitive NOESY 297, 299, 300, 302, 303, 308
 - phosphines and phosphonium salts
 - ^{31}P NMR chemical shifts of 157
 - platinum phosphite complexes
 - ^{31}P NMR data for 179

- 31P** NMR spectra 1, 2, 155–179
 Pt(0) norbornene complexes, ³¹P data for 170
 Pt(II) substituted olefin complexes 104
 Pt(LL)(CO₃) complexes 126
¹⁹⁵Pt NMR 188
 Pt(triphos) dicitations with 4-substituted pyridines and anilines – ³¹P data and pKa values for 170
 90° pulse 8
 pulsed gradient spin-echo (PGSE) 55, 56, 57, 59–60
- r**
 relaxation 9
 – chemical shift anisotropy 15–16
 – dipole–dipole relaxation 12–14
 – useful tips 16–17
 remote agostics 66, 226
 remote interaction 226
 remote olefin bonding 107
⁸¹⁰³Rh chemical shift 191, 192
 Rh(III) phenyl complexes 192
 Rh and Ir (ttp) and Cytp-type complexes, ³¹P NMR data for 172
 Rh-bis(chelate)+ and Rh(diene)(chelate)+ salts – ¹⁰³Rh NMR data for 197
 Rh-catalyzed enantioselective hydrogenation 164
¹⁰³Rh chemical shift 190
 RhCl(P(CH₃)₃)₃ 230
 Rh-CO and Rh-C(O)Et ¹³C chemical shifts 124
 Rh complexes with bidentate P donors, ³¹P NMR data for 177
 rhodium complexes, ³¹P NMR spectra of 162
 routine measuring and relaxation 7
 – getting started 7–9
 – relaxation 9
 – – chemical shift anisotropy 15–16
 – – dipole–dipole relaxation 12–14
 – – useful tips 16–17
 Ru(Cp^{*}) cation 224
 Ru(II) phosphine complexes, ³¹P chemical shifts in 168
- s**
 sample problems 319–322
 signal-to-noise (S/N) ratio 7
- sp**²-hybridized N donors 138
 spin–lattice relaxation times 5, 10
 Stokes–Einstein equation 57
- t**
 terpyridine (Terpy) iron salts 140
 tetramethylsilane (TMS) 63, 225
 trans effect 83
 trans influence and ¹J 230–238
 trans influence concept 83
 transition metal alkyl complex synthesis 316
 transition metal carbene complex synthesis 318
 transition metal carbonyl complex synthesis 317
 transition–metal–hydride complex synthesis 316
 transition metal hydrides 67
 transition metal olefin complex synthesis 317–318
 transition metals 179–196
 – olefin complexes of 4
 trans-PdCl₂(L)(phosphine), ³¹P NMR chemical shift data for 168
trans-PdCl₂(P(*n*-Pr)₃)₂ 251
trans-PdCl₂(P(*p*-Tolyl)₃)₂ 249
trans-PdCl₂(PBu₃ⁿ)₂ 249
trans-PtCl₂(η₂-C₂H₄)[(S)-N-methyl α-methyl benzylamine] 243
 tungsten imido and amido complexes 146
 two and three long-range bond ¹³C,¹H correlations 26–31
- v**
 variable temperature 280–284
¹⁸³W NMR chemical shifts 184
- x**
¹H correlations 31–36
¹H Overhauser effects 41–43
- z**
 Zr–H–C agostic alkenyl zirconium complexes 225