

Index

a

- actinides-based SMMs
 - azobenzene 13
 - mixed 3d-5f complex 15
 - mononuclear uranium(III) SMMs 13
 - polynuclear actinide complexes 14
 - spin-orbit coupling 12
 - uranium(III) scorpionate complexes 13
- adiabatic susceptibility 49, 51, 53, 56–59, 61, 63, 64, 78
- alcoholysis 26, 259, 260
- algorithms and libraries for physics
 - simulations (ALPS) project 115
 - input files 118–120
 - input structure 121
 - lattice definitions 118–119
 - model definitions 119–120
- aminoxyl 318
- amphiphilic ligands 25
- anisotropic Hamiltonian 112, 113
- Argand plot 54, 58, 61
- Arrhenius plot 74, 77, 207, 208, 210
- assisted self-assembly 274, 279

b

- benzosemiquinonoid and nindigo
 - radical SMMs 323–325
- 2,6-bis(1,1-bis(2-pyridyl)ethyl)pyridine (PY5Me₂) 283
- 1,3-bis(3-methoxy-salicylamino)-2-propanol 379
- 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine 267

- 3,6-bis(vanillidenehydrazinyl)-1,2,4,5-tetrazine 267
- Bloch walls 2
- Boltzmann distribution 49, 55, 93
- Boltzmann population 106
- 2,2-bipyrimidine (bpy_m) 338, 339
- 2,2'-bpy ligand 342
- Brillouin theory 93–94
- building-block approach 283
- (Buⁿ₄N)[Tb{Pc(OEt)₈}₂] 290

c

- carbene radical SMMs 321–323
- carbon nanostructures 20, 26
- carbon nanotubes (CNTs) 21, 326
- carboxylate substitution reactions, 254
- Casimir-Du Pre-Debye model 59, 60
- CASSCF/RASSI approach 110–112
- chlorido bridges 265–266
- [(18-C-6)K(thf)₂][(t^{bs}L)Fe₃] and [(crypt-222)K][(t^{bs}L)Fe₃] 202–203
- classical ligand-field theory (LFT) 148, 149, 168
- classical Monte Carlo (CMC) 117, 122
- classical spin Heisenberg chain equation 3
- Cobalt(II) 248, 288
- [Co^{II}₂Co^{III}₄Ln^{III}₄(HL41)₈(OAc)₆(NO₃)₄(H₂O)(MeOH)]²⁺ 370
- [Co^{II}₂Ln^{III}₄(μ₃-OH)₂(piv)₄(L12)₄(ae)₂·(NO₃)₂·2H₂O 376
- [Co^{II}₃Dy^{III}₄(μ₃-OH)₆(L22)₆(CF₃SO₃)](ClO₄)₅] 368, 373

- $[\text{Co}^{\text{II}}_3\text{Dy}^{\text{III}}_4(\mu_3\text{-OH})_6(\text{L22})_6(\text{CF}_3\text{SO}_3)(\text{ClO}_4)_5]$ (*contd.*)
 $[\text{Co}^{\text{II}}_3\text{Ln}^{\text{III}}_4(\mu_3\text{-OH})_6(\text{L22})_6(\text{CF}_3\text{SO}_4)(\text{CF}_3\text{SO}_4)_5]$ 374
 $[\text{Co}^{\text{II}}_4\text{Dy}^{\text{III}}_2(\mu_3\text{-OH})_2(\text{L43})_4\text{Cl}_2(\text{NO}_3)_2(\text{MeOH})_4]$ 375
 $[\text{Co}^{\text{II}}_4\text{Ln}^{\text{III}}_2(\mu_3\text{-OH})_2(\text{L16})_4\text{Cl}_2(\text{NO}_3)_2(\text{MeOH})_4]\cdot 3(\text{Et}_2\text{O})$ 374
 $[\text{Co}^{\text{II}}_6\text{Ln}^{\text{III}}_2(\text{OH})_4(\text{L23})_6(\text{piv})_8(\text{CH}_3\text{CN})_2]$ 379
 $[\text{Co}^{\text{III}}_2\text{Dy}^{\text{III}}_4(\text{OH})_2(\text{L11})_4(\text{OAc})_4(\text{NO}_3)_4(\text{H}_2\text{O})_2]$ 377
 $[\text{Co}^{\text{III}}_2\text{Dy}^{\text{III}}_4(\mu_3\text{-OH})_2(\text{L11})_4(\text{NO}_3)_4(\text{OAc})_4(\text{H}_2\text{O})_2]$ 376
 $[\text{Co}^{\text{III}}_4\text{Dy}^{\text{III}}_2(\text{OH})_2(\text{HL46})_2(\text{L46})_2(\text{Piv})_6]$ 377
 $[\text{Co}_2\text{Dy}_2(\text{vdpyCH}_2\text{O})_2(\text{CH}_3\text{CO}_2)_8]$ 340
 $[\text{Co}(\text{hfpip})_2(\text{D}_2\text{py}_2(\text{TBA}))_2]$ 323
 $\text{Co}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ with 4,4-dimethyl-2,2-di(2-pyridyl) oxazolidine
 N-oxide (*dmpoNO*) 338, 339
 $[\text{Co}(\text{tBu-hfpip})_2(\text{D}_2\text{py}_2(\text{TBA}))_2]$ 323
 Cole–Cole model 65, 69
 Cole–Cole plot 54, 66, 78, 375
 complex bis(η^8 -cyclooctatetraenyl) neptunium(IV) 300
 coulomb interaction 99
 crusts 251
 crystal-field Hamiltonian 99, 107
 crystal-field interaction 99, 100, 103
 crystal fields 99, 113, 289
 $[\text{Cu}_2\text{Dy}_2(\text{hfac})_{10}(\text{NIT-3py})_2(\text{H}_2\text{O})_2]$ 340
 $[\text{Cu}_3\text{Ln}_2(\text{H}_3\text{L48})_2\text{X}_n]$ 378
 $[\text{Cu}_3\text{Tb}_2(\text{hfac})_8(\text{OH})_4\text{N3tempo}]$ 342
 $[\text{Cu}_5\text{Gd}_2(\text{OH})_4(\text{H}_2\text{L})_2(\text{H}_3\text{L})_2\text{Br}_2(\text{NO}_3)_2(\text{H}_2\text{O})_4](\text{NO}_3)_2$ 277
 $[\text{Cu}_5\text{Ln}_2(\text{H}_2\text{L49})_2(\mu_3\text{-OH})_4(\mu\text{-OAc})_4]$ 379
 $[\text{Cu}^{\text{II}}_2\text{Gd}^{\text{III}}(\text{L3})_2(\text{NO}_3)_2(\text{H}_2\text{O})]\cdot \text{EtNO}_2$ 363
 $[\text{Cu}^{\text{II}}_3\text{Dy}^{\text{III}}_2(\mu_3\text{-OH})(\text{L51})(\text{HL51})_3(\text{H}_2\text{L51})(\text{MeOH})_2]\text{Br}$ 379
 $[\text{Cu}^{\text{II}}_4\text{Ln}^{\text{III}}_2(\text{L5})_4(\text{OH})_2(\text{NO}_3)_4(\text{H}_2\text{O})]$ 363
 $[\text{Cu}^{\text{II}}_5\text{Dy}^{\text{III}}_5(\mu_4\text{-O})(\mu_3\text{-OH})_3(\text{L52})_3(\text{HL52})_4(\text{NO}_3)_2(\text{MeOH})_2]$
 $[\text{Cu}^{\text{II}}_5\text{Dy}^{\text{III}}_5(\mu_4\text{-O})(\mu_3\text{-OH})_3(\text{L52})_3(\text{HL52})_4(\text{NO}_3)(\text{MeOH})_3(\text{H}_2\text{O})](\text{NO}_3)\text{H}_2\text{O}\cdot 25\text{MeOH}$ 379
 $[\text{Cu}^{\text{II}}_6\text{Ln}^{\text{III}}_3(\text{L34})_6(\text{OH})_6(\text{H}_2\text{O})_{10}]^{3+}$ 370
 $[\text{Cu}^{\text{II}}_9\text{Dy}^{\text{III}}_2(\mu_3\text{-OH})_4(\mu_3\text{-Br})_2(\text{L50})_2(\text{HL50})_4(\text{Br})_2(\text{NO}_3)_2(\text{MeOH})_4]$ 379
 $[\text{Cu}^{\text{II}}\text{Gd}^{\text{III}}(\text{L4})_2(\text{H}_2\text{O})_3][(\text{Cu}^{\text{II}}(\text{L4}))(\text{ClO}_4)]$ 363
 Curie's law susceptibility equation 94
 cyanide-bridged complexes 231–233
 cyano-bridged 3d/*nd* ($n=4,5$) SMMs 283
d
 DC susceptibility measurements 122
 Debye equation 53, 57
 Debye model 53, 58, 176
 Debye relaxation model 54, 55, 57, 63
 $[\text{dmp}_2\text{Nin}[\text{Co}(\text{N}\{\text{SiMe}_3\}_2)_2(\text{Et}_2\text{O})_2]^+]$ 325
 $[\text{dmp}_2\text{Nin}[\text{Co}(\text{N}\{\text{SiMe}_3\}_2)_2]^-]$ 325
 density functional theory (DFT) 90, 127–130, 259, 267, 272, 290, 337, 356, 368
 denticity 283
 diamagnetic MOF 27
 dianionic ligands 199, 293
 DiAn program 358
 didiazo-dipyridine ligand $\text{D}_2\text{py}_2(\text{TBA})$ 323
 differential magnetic permeability 44
 dihedral angle 221, 291, 337
 dimers 75, 89, 111–113, 143, 144, 266, 268, 269
 1,5-dimethyl-3-[6'-(hydroxymethyl)-2'-pyridine]-6-oxotetrazane ($\text{H}_3\text{vdpyCH}_2\text{OH}$) 340
 dinuclear Ln(III) compounds 262
 dinuclear/polynuclear uranium system 272
 dodecanuclear manganese mixed valence compound 354

- domains algorithm 362
double exchange 184, 200, 202
Dy complex 24, 27, 229, 342
[Dy(O^tBu)₂(Py)₅](BPh₄) complex 291
[DyI{fc(NSi^tBuMe₂)₂}(THF)₂] complex 293
[Dy(hfac)₃{NITPy}]₂ 335
[Dy₂Cl₂(ovph)₂(MeOH)₃] 264
[Dy₂(hfac)₄(NITPhO)₂] 336
dysprosium metallocene unit 16
- e**
electric field gradient (EFG) 178, 179, 206
electromotive force (EMF) 70–72
enantioselectivity 28
enhanced toroidal moment compounds 6
exchange coupling 6, 12, 75, 76, 103, 105, 110–115, 125, 126, 180, 196, 232, 247, 265, 269, 270, 273, 283, 285
- f**
far-infrared magnetic resonance spectroscopy (FIRMS) 147
[Fe(CN)₆]³⁻ unit 232
[Fe₄Dy₂(μ₄-O)₂(NO₃)₂(piv)₆(Hedte)₂].4MeCN·C₆H₅OH 223–224
[Fe₇Dy₃(μ₄-O)₂(μ₃-OH)₂(mdea)₇(μ-benzoate)₄(N₃)₆].2H₂O·7MeOH 222–223
[Fe^I(cAAC)₂][B(C₆F₅)₄] 212–213
[Fe^I(cAAC)₂Cl] 211–213
[Fe^{II}(Eind)₂] 214–215
[Fe^{II}{C(SiMe₃)₃}]₂ 207–209, 287
[Fe^{II}{N(SiMe₃)(Dipp)}₂] 209–210
[Fe^{II}{N(SiMe₃)₂}(PCy₃)] 287
[Fe^{II}{O(C₆H₃-2,6-(C₆H₃-ⁱPr)₂)₂}] 210–211
[Fe^{II}₂(acpyentO)(NCO)₃] 195–196
[Fe^{II}₂Dy(L)₂(H₂O)](ClO₄)₂·2H₂O 230–231
[Fe^{II}₇(OMe)₆(Hbmsae)₆]Cl₂·6H₂O 197–199
[Fe^{II}₉(X)₂(O₂CMe)₈{(2-py)₂CO₂}]₄ 196–197
[Fe^IFe^{III}(L)(O₂CMe)₂](ClO₄) 199–201
{Fe^{III}[Fe^{III}(L¹)₂]}₃ 194–195
[Fe^{III}₁₁O₇(dea)₃(piv)₁₂]Cl·5MeCN 189–190
[Fe^{III}₂Dy₂(μ₃-OH)₂(pmide)₂(*p*-Me-C₆H₅CO₂)₆] 225
[Fe^{III}₂Dy₂(μ₃-OH)₂(teg)₂(N₃)₂(C₆H₅CO₂)₄] 224–225
[Fe^{III}₂Dy^{III}₂(OH)₂(L¹)₂(HL²)₂(NO₃)₄(H₂O)_{1.5}(MeOH)_{0.5}].6MeCN 225–228
[Fe^{III}₂Ln₂(H₂L)₄(NO₃)₂](ClO₄)₂·2MeOH·2H₂O 228–229
[Fe^{III}₂Ln^{III}₂(OH)₂(teaH)₂(O₂CCPh)₆].3MeCN 217–218
[Fe^{III}₃Ln(μ₃-O)₂(CCl₃CO₂)₈(H₂O)(thf)₃].*x*(thf)·*y*(heptane) 229–230
[Fe^{III}₄(OMe)₆(dpm)₆] 191–194, 234
[Fe^{III}₄Dy^{III}₂(OH)₂(*n*-bdea)₄((CH₃)₃CCO₂)₆(N₃)₂].3MeCN 221–222
[Fe^{III}₄Dy^{III}₂(OH)₂(*n*-bdea)₄(C₆H₅CO₂)₈].MeCN 219–220
[Fe^{III}₄Dy^{III}₄(teaH)₈(N₃)₈(H₂O)].H₂O·4MeCN 215–217
[Fe^{III}₄Ln^{III}₂(teaH)₄(N₃)₇(piv)₃] 218–219
[Fe^{III}₈O₂(OH)₁₂(tacn)₆][Br₈·9H₂O] 185–187
- Fe/4f single molecule magnets
[Fe₄Dy₂(μ₄-O)₂(NO₃)₂(piv)₆(Hedte)₂].4MeCN·C₆H₅OH 223–224
[Fe₇Dy₃(μ₄-O)₂(μ₃-OH)₂(mdea)₇(μ-benzoate)₄(N₃)₆].2H₂O·7MeOH 222–223
[Fe^{II}₂Dy(L)₂(H₂O)](ClO₄)₂·2H₂O 230–231
[Fe^{III}₂Dy₂(μ₃-OH)₂(pmide)₂(*p*-Me-C₆H₅CO₂)₆] 225
[Fe^{III}₂Dy₂(μ₃-OH)₂(teg)₂(N₃)₂(C₆H₅CO₂)₄] 224–225
[Fe^{III}₂Dy^{III}₂(OH)₂(L¹)₂(HL²)₂(NO₃)₄(H₂O)_{1.5}(MeOH)_{0.5}].6MeCN 225–228
[Fe^{III}₂Ln₂(H₂L)₄(NO₃)₂](ClO₄)₂·2MeOH·2H₂O 228–229

- Fe/4f single molecule magnets (*contd.*)
 $[\text{Fe}^{\text{III}}_2\text{Ln}^{\text{III}}_2(\text{OH})_2(\text{teaH})_2(\text{O}_2\text{CCPh})_6] \cdot 3\text{MeCN}$ 217–218
 $[\text{Fe}^{\text{III}}_3\text{Ln}(\mu_3\text{-O})_2(\text{CCl}_3\text{CO}_2)_8(\text{H}_2\text{O})(\text{thf})_3] \cdot x(\text{thf}) \cdot y(\text{heptane})$ 229–230
 $[\text{Fe}^{\text{III}}_4\text{Dy}^{\text{III}}_2(\text{OH})_2(n\text{-bdea})_4((\text{CH}_3)_3\text{CCO}_2)_6(\text{N}_3)_2] \cdot 3\text{MeCN}$ 221–222
 $[\text{Fe}^{\text{III}}_4\text{Dy}^{\text{III}}_2(\text{OH})_2(n\text{-bdea})_4(\text{C}_6\text{H}_5\text{CO}_2)_8] \cdot \text{MeCN}$ 219–220
 $[\text{Fe}^{\text{III}}_4\text{Dy}^{\text{III}}_4(\text{teaH})_8(\text{N}_3)_8(\text{H}_2\text{O}) \cdot \text{H}_2\text{O} \cdot 4\text{MeCN}$ 215–217
 $[\text{Fe}^{\text{III}}_4\text{Ln}^{\text{III}}_2(\text{teaH})_4(\text{N}_3)_7(\text{piv})_3]$ 218–219
- Foner-type vibrating-sample magnetometer 7
- 4f metal radical SMMs
 2,2-bipyrimidine (bpym) 338, 339
 nitroxide radical SMMs 331–336
 N_2^{3-} radical SMMs 336–338
 phthalocyanine radical SMMs 325–331
 tetra-2-pyridinylpyrazine (tppz) 338–340
- 4f-metal SIMs synthesis
 non-phthalocyanine 291–296
 phthalocyanine-based 290–291
- 4f-metal SMMs synthesis
 chlorido bridges 265–266
 dinuclear Ln(III) compounds 262
 monoatomic and polyatomic N-based ligands 266–267
 multidecker
 lanthanide(III)-phthalocyanine SMMs 270–271
 O-bridged groups 264–265
 organometallic bridges 267–268
 radical-bridged lanthanide(III) SMMs 268–270
 sulfur-bridged SMMs 267
 tunneling 262
- 4f/5f-metal clusters and SMMs synthesis 281–282
- 5f metal radical SMMs 342–343
 5f-metal SIMs synthesis 296–301
 5f-metal SMMs synthesis 271–273
- Fourier-transform infra-red (FTIR) spectroscopy 147
 frequency-domain Fourier-transform terahertz-EPR (FD-FT THz-EPR) 147
- g**
 gadolinium-based agents 25
 $[\text{Gd}(\text{NITBzImH})_4]^{3+}$ 332
 $[\text{Gd}(\text{NITMeBzImH})_4]^{3+}$ 332
 Gd^{III} nitroxide compounds 332
 gearwheel-like molecular structures 122
 giant spin approximation 139, 180
 giant-spin Hamiltonian 138
 Gibbs thermodynamics potential 48
 graphene 21, 22, 326
- h**
 Hamiltonian approximation 180
 Hamiltonian matrix 89, 105, 108, 127
 hard and soft acids and bases (HSAB) 267, 274, 287, 295, 363
 harmonic complex magnetic ac susceptibility 72
 Harris notation 247, 249
 Hartshorn bridge 69, 70, 78
 Heaviside step function 51
 Heisenberg–Dirac–VanVleck effective Hamiltonian 105
 Heisenberg model 87
 Helmholtz potential 48
 heptanuclear cluster 277
 hexadecanuclear cycle 124
 hexanuclear complex 108
 $[\text{HFe}^{\text{III}}_{19}\text{O}_{14}(\text{OEt})_{30}]$ 190–191
 high-field electron paramagnetic resonance (HFEP) resonance (HFEP)
 alternative techniques 146–147
 dimers 143–144
 energy levels 137
 limitations 146
 magnetization hysteresis loops 136
 mononuclear transition metal complexes 144–146
 polycrystalline powder spectra 136
 polynuclear clusters 143

- powder-pattern spectrum 136, 137
 quantum tunneling effects 136
 recapitulation 167–169
 spin Hamiltonian
 3A_2 and $^3E_{(b)}$ excited states 163
 3B_2 and $^3E_{(a)}$ excited states 160
 3B_2 wavefunction 200
 classical ligand-field theory (LFT) 148
 contribution from $^3E_{(a)}$ 161
 correlation diagram 149
 d^2 basis set 165
 effect of 139, 140
 electronic spin system 159
 energy splitting 167
 excited state wavefunctions 166
 ground state 150
 ground state wavefunction 166
 high-spin mononuclear transition metal complexes 140
 homoleptic complexes 149
 interelectronic repulsion
 parameters 148
 interpretation 138
 nephelauxetic effect 148
 non-zero matrix elements 151, 152
 non-zero matrix elements between $^3E_{(b)}$ and 3B_1 163
 orbital angular momentum operators 151, 155
 perturbation method 149
 quantum chemical calculations 148
 Racah interelectronic repulsion parameter 165
 second order perturbation theory 154, 158, 164, 166
 single-electron orbital angular momentum operator 151, 152
 singlet excited state 150, 151
 singlet excited states 159
 Slater determinants 149
 SOC 139
 SOC Hamiltonian 149, 151
 spectroscopic Landau factor 139
 spin angular momentum operator 151
 spin quartet Kramers system 139
 spin raising/lowering operator 152
 spin-spin contributions 148
 spin triplet non-Kramers species 139
 Stevens operators 139
 3T_1 states 159
 $^3T_{2(a)}$ and $^3T_{2(b)}$ wavefunctions 159
 $^3T_{2(b)}$ wavefunctions 156
 tetrahedral parent complex 163
 tetrahedral splitting 167
 triplet electronic states 160
 unquenched orbital angular momentum 139
 wavefunction 151
 Zeeman effect 140, 141
 Zeeman interaction 139
 ZFS 139, 166, 167
 ZFS 136
 high-field EPR 146, 236
 homogeneous external magnetic field 46
 HvdpyCH₂OH²⁻-verdazyl radical 340
 (2-[(3-hydroxy-ethylimino)-methyl]-6-methoxy-phenol) 370
 (2-[(3-hydroxy-propylimino)-methyl]-6-methoxy-phenol) 370
 hyperfine interactions, Mössbauer spectroscopy
 isomer shift 176–178
 magnetic hyperfine interactions 179–180
 quadrupole splitting 178–179
- i**
- inelastic neutron scattering (INS) 147, 168, 234–236
 in-phase susceptibility 50
 inter-Kramers transitions 141, 146
 intermolecular interactions 13, 18, 19, 73–78, 189, 247, 316, 327, 329, 343

- iron(III) ions 121, 188–190, 194, 229
- irreducible tensor operators (ITO) 89, 107–108
- Ising chain equation 3
- Ising-type lanthanide molecular clusters 5
- IsoCryst program 361
- isomer shift 176–178, 183, 190, 193, 196–198, 200, 202, 206, 208, 210–213, 215, 216, 218, 220–222, 233
- isostructural cationic complexes 17
- isostructural [LaFe] and [CeCo] systems 113, 114
- isostructural TiOPc matrix 20
- isothermal and adiabatic susceptibilities 49, 63
- isothermal susceptibility 51, 53, 56, 58
- j**
- Jahn–Teller distortion 5, 248, 283, 286
- Jahn–Teller isomerism 9, 21, 253
- k**
- [K(18C6)(THF)₂][Dy(BIPM^{TMS})₂] 294
- [K(18-crown-6)]{[(Me₃Si)₂N]₂(THF)Ln]₂(μ-η²:η²-N₂)} 336
- [K(crypr-222)][Fe^I{C(SiMe₃)₃]₂] 207–208
- [K(L)][Fe^I{N(SiMe₃)₃]₂] 213–214
- K[[(SiMe₃)N]₂(THF)Ln]₂(μ₃-η²:η²-N₂) 336
- Kramers systems 137, 146
- Kronig–Kramers relations 45
- l**
- Lamb–Mössbauer factor 175
- Lande *g*-factor 91–92
- lanthanide-based SIMs 4, 5
- Legendre transformation 48
- linear 2-coordinate geometry, Kramers's system 287
- Lines model 110
- [Ln(hfac)₃NIT-2Py] 332
- [Ln(L)₃(NIT-2Py)] 333
- [Ln(Pc)₂] radical 325–327
- [Ln(tfa)₃(NIT-BzImH)] 333
- long range ordering 182, 247
- L*-*S*-coupling 95–99
- L*-*S* multiplets 95, 96
- m**
- MagLab 169
- magnetic ac-susceptibility 42
- adiabatic susceptibility 59
- Argand diagram 58, 61
- coercive field and remanence magnetization 55
- Cole-Cole and Davidson-Cole models 61
- Cole-Cole equation 59
- Cole-Cole plot 54
- Cole-Cole type distribution 61
- complex ac susceptibility 50
- complex susceptibility 57
- constant magnetization and magnetic field 58
- Debye equations 53
- definition 49
- demagnetization effects 51
- electromagnetic definitions 43–45
- external ac magnetic field 49
- ferromagnetically coupled triangular Cu₃ complex 69
- induced ac magnetization 49
- in-phase susceptibility 50
- intermolecular interactions 73–78
- isothermal susceptibility 51, 53
- magnetic ellipsoid 46
- magnetic moment 56
- magnetic susceptibility 49
- magnetization 50, 56
- adiabatic magnetization 53
- equilibrium magnetization 52
- exponential approach 52
- harmonic external magnetic field 54
- time variation 51, 52
- total magnetization 53
- magnetostatic energy 45–47
- non-zero adiabatic susceptibility 61
- nth order harmonic complex 50

- one-dimensional chain based on Mn_6 units 64–69
- Orbach process 52
- out of phase susceptibility 50
- polynuclear transition molecules 62
- Raman process 52
- real and imaginary part 57
- relaxation time 42, 43, 51, 52, 55, 58, 59, 62
- single-ion complexes 43
- spin-lattice relaxation time 57
- spin temperature 56
- technical aspects 69–73
- thermodynamic equilibrium 49
- thermodynamic relations 48–49
- time dependent perturbation theory 51
- tris(acetylacetonato) iron(III) ($Fe(acac)_3$)
 - Argand diagram 63, 64
 - dc-magnetic field and frequency 63
 - electron paramagnetic resonance studies 63
 - relaxation rate 65
- zero-field splitting 62
- magnetic ellipsoid 46
- magnetic enthalpy 48–49
- magnetic entropy 23, 24, 106
- magnetic field
 - analysis 46
 - Brillouin theory 93–94
 - crystal fields 99
 - energy spectrum
 - many electrons case 95
 - single electron case 94
 - free atoms
 - diamagnetic contribution 92
 - Hamiltonian 90
 - Lande g -factor 91–92
 - magnetic moment 92
 - polarization contribution 92
 - second order perturbation theory 90
 - van Vleck paramagnetic term 92
 - Zeeman energy 91, 92
 - Zeeman interaction 91
 - single-ion anisotropy 100
- magnetic hyperfine interactions 179–180
- magnetic induction 43–47, 55, 56, 71, 72
- magnetic modelling
 - Monte Carlo simulations 115
 - PHI v.3.0
 - anisotropic exchange coupling 110–115
 - general Hamiltonian 103
 - Hamiltonian formalism, exchange coupling 105
 - isotropic case 108–110
 - ITO method 107–108
 - thermodynamic properties 106–107
- magnetic refrigeration 23–25, 366
- magnetic relaxation
 - characteristic time 182
 - Dc magnetization measurements 181
 - electronic spin 181
 - long range ordering 182
 - mixed valence systems 183–184
 - size distribution 182
 - spin-lattice relaxation mechanism 182
 - temperature variation 182
 - total relaxation time 182
- magnetic susceptibility 106, 189, 192, 194–196, 198–200, 202, 203, 205, 207–209, 211–214, 216–218, 223, 229, 232, 236
- magnetic susceptibility tensor 44, 45
- magnetization 2–5, 7, 9, 11, 13, 14, 17, 18, 23, 25, 42–51, 53, 55, 62, 66, 70–73, 92, 94, 102, 103, 106, 113, 122, 136, 147, 189, 194, 196, 205, 213, 247, 260, 273, 321, 322, 325, 326, 329, 333, 336, 338, 342
- magnetocaloric effect (MCE) 23, 373
- magnetometric methods 147
- Markov chain Monte Carlo scheme 117
- $[M(CN)_6]^{3-}$, paramagnetic hexacyanidometallates(III) 231
- Meppz²⁻groups 124

- $(((\text{Me}_3\text{Si})_2\text{N})_2(\text{THF})\text{Ln})_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-N}_2)$
 11
 metal complexes as ligands approach
 274, 275
 $[(\text{Me}_3\text{TPyA})_2\text{Fe}^{\text{II}}(\text{L})](\text{BARF}_4)_2$ and
 $[(\text{Me}_3\text{TPyA})_2\text{Fe}^{\text{II/III}}_2(\text{L})]$
 $(\text{BARF}_4)_3\cdot\text{CH}_2\text{Cl}_2$ 201–202
 metalloligands 274–276, 283
 metal nanoparticles 25
 metal-organic frameworks (MOFs) 27,
 356
 micellar polymeric particles 25
 microscopic spin Hamiltonian 138
 mixed (phthalocyaninato)
 (porphyrinato)lanthanide(III)
 complexes 291
 mixed valence systems 183–184
 1,1,2,4,5M10-1 motif 368–369
 2,3,3,5,5,7M10-1 motif 369, 370
 2,3,4,4M10-1 motif 369, 370
 2,3,4M6-1 motif 369, 370, 374–377
 2,4M8-1 motif 377
 3,4,6M8-2 motif 379
 $[\text{M}_6\text{Ln}_6(\text{NO}_3)_6(\text{L47})_{12}(\text{H}_2\text{O})_x$
 $(\text{MeCN})_y]$ 378
 $[\text{Mn}_{12}]$ molecule 9, 21, 25
 $[\text{Mn}^{\text{II}}_2\text{Ln}^{\text{III}}_4(\text{L45})_2(\mu_3\text{-OH})_4(\mu_3\text{-piv})_4]\cdot$
 $3\text{MeCN}\cdot 7\text{MeOH}\cdot\text{H}_2\text{O}$ 376
 $\{[\text{Mn}^{\text{III}}(\text{salphen})(\text{MeOH})]_2\text{M}^{\text{III}}(\text{CN})_6\}$.
 7MeOH 285
 $[\text{Mn}^{\text{III}}_3\text{O}(\text{O}_2\text{CMe})_6(\text{Him})_3](\text{O}_2\text{CMe})$
 cluster 259
 $[\text{Mn}^{\text{III}}_6\text{Ln}^{\text{III}}_4(\text{L39})_6(\text{H}_2\text{L39})_2(\text{L40})_2$
 $(\text{OH})_2(\text{OAc})_4(\text{MeOH})_8]$ 368
 $[\text{Mn}^{\text{III}}_{12}\text{Mn}^{\text{IV}}_9\text{O}_{24}(\text{OMe})_8$
 $(\text{O}_2\text{CCH}_2\text{Bu}^t)_{16}(\text{H}_2\text{O})_{10}]$ cluster
 259
 $[\text{Mn}^{\text{III}}_{84}\text{O}_{72}(\text{OH})_6(\text{OMe})_{24}(\text{O}_2\text{CMe})_{78}$
 $(\text{MeOH})_{12}(\text{H}_2\text{O})_{42}]$ cluster 260
 $[\text{Mn}^{\text{IV}}_4\text{Mn}^{\text{III}}_8\text{O}_{12}(\text{OAc})_{16}(\text{H}_2\text{O})_4]$ 354,
 361
 modify adjacency matrix 361
 modular process 283
 molar susceptibility 106
 MOLCAS package 110
 molecular magnets, characteristics 42
 molecular nanomagnets 20, 77, 269
 monoatomic and polyatomic N-based
 ligands 266–267
 monodentate tricyclohexylphosphine
 287
 monometallic dysprosium complex 5
 mononuclear 6-coordinated Ln(III)
 complexes 275–276
 mononuclear single-molecule magnets
 (MSMM) 4, 179
 Monte Carlo simulations
 ALPS project 115, 118
 heterometallic molecular wheels
 crystallographic description 121,
 122
 magnetic description 122, 123
 structure 122
 temperature dependence 123
 high-nuclearity copper cages
 crystallographic description 124
 cupric salts reaction 123
 magnetic description 124–126
 local vs. non-local updates 117–118
 $\text{Mn}^{\text{III}}_6\text{Mn}^{\text{II}}_6$ molecular wheel case
 B3LYP functional 127, 128
 DFT methods 127
 Gaussian basis 127
 Jahn-Teller distorted geometries
 127
 magnetic model 128
 nanocage Fe_{42} 128–130
 PBE functional 127
 multi-walled carbon nanotubes
 (MCNTs) 21
 quantum lattice models 115
 SSE algorithm 115–117
 thermalization process 118
 Moore's law 12, 20
 Mössbauer spectroscopy 168, 211, 231
 basic principles 175, 176
 cyanide-bridged complexes 231
 $[(18\text{-C-6})\text{K}(\text{thf})_2][(\text{t}^{\text{bs}}\text{L})\text{Fe}_3]$ and
 $[(\text{crypt-222})\text{K}][(\text{t}^{\text{bs}}\text{L})\text{Fe}_3]$
 202–203
 $[\text{Fe}^{\text{I}}(\text{cAAC})_2][\text{B}(\text{C}_6\text{F}_5)_4]$ 212–213
 $[\text{Fe}^{\text{I}}(\text{cAAC})_2\text{Cl}]$ 211–212
 $[\text{Fe}^{\text{II}}\{\text{C}(\text{SiMe}_3)_3\}_2]$ 208–209
 $[\text{Fe}^{\text{II}}\{\text{N}(\text{SiMe}_3)(\text{Dipp})\}_2]$ 209–210

- $[\text{Fe}^{\text{II}}\{\text{O}(\text{C}_6\text{H}_3\text{-}2,6\text{-}(\text{C}_6\text{H}_3\text{-}i\text{Pr}_2)_2)_2\}]$
 210–211
 $[\text{Fe}^{\text{II}}(\text{acpyptentO})(\text{NCO})_3]$ 195–196
 $[\text{Fe}^{\text{II}}_7(\text{OMe})_6(\text{Hbmsae})_6]\text{Cl}_2\cdot 6\text{H}_2\text{O}$
 197–199
 $[\text{Fe}^{\text{II}}_9(\text{X})_2(\text{O}_2\text{CMe})_8\{(2\text{-py})_2\text{CO}_2\}_4]$
 196–197
 $[\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}(\text{L})(\text{O}_2\text{CMe})_2](\text{ClO}_4)$
 199–201
 $\{\text{Fe}^{\text{III}}[\text{Fe}^{\text{III}}(\text{L}^1)_2]\}_3$ 194–195
 $[\text{Fe}^{\text{III}}_{11}\text{O}_7(\text{dea})_3(\text{piv})_{12}]\text{Cl}\cdot 5\text{MeCN}$
 189–190
 $[\text{Fe}^{\text{III}}_4(\text{OMe})_6(\text{dpm})_6]$ 191–194
 $[\text{Fe}^{\text{III}}_8\text{O}_2(\text{OH})_{12}(\text{tacn})_6]\text{Br}_8\cdot 9\text{H}_2\text{O}$
 185–187
 $[\text{HFe}^{\text{III}}_{19}\text{O}_{14}(\text{OEt})_{30}]$ 190–191
 hyperfine interactions 176
 $[\text{K}(\text{crypr-}222)][\text{Fe}^{\text{I}}\{\text{C}(\text{SiMe}_3)_3\}_2]$
 207–208
 $[\text{K}(\text{L})][\text{Fe}^{\text{I}}\{\text{N}(\text{SiMe}_3)_3\}_2]$ 213–214
 $[\text{M}(\text{solv})_n][(\text{tpa}^{\text{R}})\text{Fe}^{\text{II}}]$ 204–207
 $[(\text{Me}_3\text{TPyA})_2\text{Fe}^{\text{II}}(\text{L})](\text{BAR}^{\text{F}}_4)_2$ and
 $[(\text{Me}_3\text{TPyA})_2\text{Fe}^{\text{III}/\text{III}}_2(\text{L})](\text{BAR}^{\text{F}}_4)_3$
 $\cdot \text{CH}_2\text{Cl}_2$ 201–202
 Mössbauer effect 175
 $(\text{pyrH})[\text{Fe}^{\text{III}}_{13}\text{O}_4\text{F}_{24}(\text{OMe})_{12}]\cdot 4\text{H}_2\text{O}$
 $\cdot \text{MeOH}$ 187–189
 relaxation phenomena and dynamics
 181–184
 $[\text{M}(\text{solv})_n][(\text{tpa}^{\text{R}})\text{Fe}^{\text{II}}]$ 204–207
 $[(\mu_5\text{-dcp})\text{-}(\mu_4\text{-dcp})\text{-}\text{CuDy}_2(\mu_4\text{-SO}_4)$
 $(\text{H}_2\text{O})_3]\cdot \text{H}_2\text{O}$ 363
 multidecker
 lanthanide(III)-phthalocyanine
 SMMs 270–271
- n**
- nanomagnets 20, 74, 269
 National High Magnetic Field
 Laboratory (NHMFL) 169
 $(\text{NBu}_4)[\text{Tb}(\text{Pc})_2]$ 326
 nephrogenic systemic fibrosis 25
 $[\text{Ni}(\text{mpko})_2(\text{mpkoH})]$ complex 275
 $[\text{Ni}_{12}(\text{O}_2\text{CMe})_{12}(\text{chp})_{12}(\text{THF})_6(\text{H}_2\text{O})_6]$
 cluster 250
 $[\text{Ni}_4\text{Ln}_4(\text{H}_3\text{L}20)_4(\mu_3\text{-OH})_4(\mu_2\text{-OH})_4]$
 $4\text{Cl}\cdot x\text{H}_2\text{O}\cdot y\text{CHCl}_3$ 377
 nitroxide and verdazyl radicals 340
 N,N' -bis(salicylidene)-1,2-diamino
 benzene 285
 non-Kramers systems 137, 140
 non-steroidal anti-inflammatory drug
 (NSAID) 109
 non-zero adiabatic susceptibility 57,
 58, 61
 $[\text{Np}(\text{COT})_2]$ 300
 $[\text{Np}^{\text{VI}}\text{Np}^{\text{V}}_2\text{O}_6(\mu\text{-Cl})_2\text{Cl}_2(\text{THF})_6]$,
 273
 nuclear magnetic resonance (NMR) 2,
 179, 234, 235
- o**
- O-bridged groups 264–265
 1,4,8,11,15,18,22,25-octakis-fluoro-2,
 3,9,10,16,17,23,24-octakisper-
 fluoro(isopropyl)phthalocyanine
 ligand 328–329
 one-pot approach 274, 277
 "open" pentadentate chelating N_5 ligand
 283
 Orbach process 52, 192
 orbital contribution 4, 92, 180, 207,
 210, 286
 organic radicals 316
 antiferromagnetic (AF) interactions
 317
 definition 316
 polychlorotriphenylmethyl radical
 (PTM) 316, 317
 spin Hamiltonian equation 317
 triphenylmethyl radical 316
 organometallic bridges 267–268
 out of phase susceptibility
 50, 213, 223
- p**
- Pacman ligands 281
 paramagnetic
 hexacyanidometallates(III)
 231, 232
 paramagnetic MOF 27
 paramagnetic relaxation effect 19
 Pauli principle 95, 96
 permeability tensors 44

- phenomenological Hamiltonians 87
 phloroglucyl backbone 17, 18
 phosphine-oxide and phenol
 fuctionalized nitroxide radicals
 336
 (Ph₄P)₂[Co^{II}(SPh)₄] 288
 phthalocyanine 11, 16, 123, 270, 271,
 290–296, 317, 325–331
 phthalocyanine (Pc) radical SMMs
 325–331
 polarized neutron diffraction (PND)
 235
 polychlorotriphenylmethyl radical
 (P₃TM) 316, 317
 polynuclear actinide complexes
 14
 polynuclear coordination clusters
 (PCCs)
 assembly 362–363, 368–373
 bridged representation 362
 3d-4f PCCs 363
 dodecanuclear manganese mixed
 valence compound 354
 skeleton representation 362
 synthetic aspects 377–380
 targeting the 2,3,4M6-1 core
 374–376
 targeting the 3,6M7-1 core
 373–374
 topological methods 356
 polynuclear metal complexes
 25, 359
 polyoxometalate (POM)-based SMMs
 18
 pseudospin magnetic Hamiltonians
 110
 pseudotetrahedral Co(II) complexes
 289
 [(PY5Me₂)₄Mn^{II}₄Re^{III}(CN)₇](PF₆)₄,
 284
 (pyrH)[Fe^{III}₁₃O₄F₂₄(OMe)₁₂]-4H₂O·
 MeOH 187–189
 2-(4-pyridyl)-4,4,5,5-tetramethyl-4,5-
 dihydro-1H-imidazolyl-3-oxide
 (NIT4Py) 335
 2-(3-pyridyl)-4,4,5,5-tetramethylimida-
 zoline-1-oxyl-3-oxide 340
- q**
 QMC simulation process 126
 quadrupole splitting 178–179, 190,
 193, 198, 202, 206, 208, 212,
 213, 215, 217, 218, 220–222,
 233
 quantum chemical theory (QCT) 166
 quantum-classical nanoparticle
 interface 26
 quantum coherence 19, 20
 quantum computing 2, 5, 19–21, 64,
 73
 quantum dots 25
 quantum lattice model 89, 115, 117,
 118
 quantum mechanical coupling 260
 quantum Monte Carlo (QMC) study
 89, 116, 122
 quantum phase interference 73, 235,
 248
 quantum tunneling of magnetization
 (QTM) 4, 5, 13, 15, 17, 73, 205,
 247, 322
 quantum Turing machine 19
 quinoline 26, 289
- r**
 Racah interelectronic repulsion
 parameter 165
 Racah parameters 148, 165
 radical-bridged lanthanide(III) SMMs
 268–270
 Raman mechanism 5
 Raman process 52
 recoilless factor 175
 reductive aggregation 253, 260
 relaxation time 4, 5, 13, 18, 19, 42, 43,
 49, 51, 52, 54, 55, 57–59, 61–67,
 69, 74, 76, 181–183, 185, 200,
 205, 206, 218–220, 223, 224, 235,
 264, 270, 273
- s**
 salicylaldoximate ligands 108
 Schiff-base ligands 364, 365, 368, 379
 second order Doppler effect 177
 serendipitous assembly 363, 364

- simplify adjacency matrix 361
- single chain magnetism (SCM)
 - behaviour 2–4, 318
- single-crystal X-ray crystallography 256
- single-domain magnetic particle
 - behaviour 73
- single-ion anisotropy
 - angular momentum operators 100
 - axis anisotropy 103
 - crystal-field anisotropy 100
 - diagonal crystal-field parameters 101, 102
 - electrostatic interaction of charge 100
 - hard axis–easy plane anisotropy 103
 - heavy rare-earths case 100
 - interaction energy 100
 - Kramer's theorem 102
 - 2^n -pole moments 101
 - quadrupole moment 100
 - rare-earth ions 104
 - Stevens operators 101
 - susceptibility 103
- single-ion magnets (SIMs) 4–5
 - classification/evaluation 168
 - $[\text{Fe}^{\text{I}}(\text{cAAC})_2\text{Cl}]$ 211–213
 - $[\text{Fe}^{\text{II}}(\text{Eind})_2]$ 214–215
 - $[\text{Fe}^{\text{II}}\{\text{C}(\text{SiMe}_3)_3\}_2]$ 207–209, 287
 - $[\text{Fe}^{\text{II}}\{\text{N}(\text{SiMe}_3)(\text{Dipp})\}_2]$ 209–210
 - $[\text{Fe}^{\text{II}}\{\text{N}(\text{SiMe}_3)_2(\text{PCy}_3)\}]$ 287
 - $[\text{Fe}^{\text{II}}\{\text{O}(\text{C}_6\text{H}_3-2,6-(\text{C}_6\text{H}_3-^i\text{Pr}_2)_2\}_2]$ 210–211
 - 4f-metal synthesis 290–291
 - 5f-metal synthesis 296–301
 - $[\text{K}(\text{crypt-222})][\text{Fe}^{\text{I}}\{\text{C}(\text{SiMe}_3)_3\}_2]$ 207–208
 - $[\text{K}(\text{L})][\text{Fe}^{\text{I}}\{\text{N}(\text{SiMe}_3)_3\}_2]$ 213–214
 - $[\text{M}(\text{solvent})_n][(\text{tpa}^{\text{R}})\text{Fe}^{\text{II}}]$ 204–207
 - properties 141, 142
 - recapitulation 167, 169
 - 3d-metal SIMs synthesis 286
- single-molecule magnets (SMMs) 247
 - actinides 12–15
 - applications 25–28
 - bottom-up approach 12
 - classification/evaluation 168
 - Fe-based 168
 - Heisenberg model 87
 - heteronuclear Fe/4f clusters 215
 - historical aspects
 - cationic complex 9
 - dodecanuclear mixed-valence 6
 - magnetic anisotropy 10
 - magnetic properties 7, 9
 - milestones 6, 7
 - $[\text{Mn}_{12}]$ complex 9
 - Mn–O bonds 10
 - mononuclear SMM 10, 11
 - oxime ligands 10
 - phthalocyanine ligands 11
 - radical-bridged 4f complexes 11
 - radical-bridged terbium complex 12
 - salicylaldoxime ligands 10
 - superparamagnets 9
 - two-coordinate low-valent iron(I) compound 11
 - inelastic neutron scattering (INS) 235, 236
 - magnetic domain 2
 - magnetic field 90
 - magnetic macromaterials 2
 - magnetic modelling 103
 - magnetic molecules 2, 12
 - magnetic properties 89
 - magnetic refrigeration 23
 - metal radical 316
 - 3d 318
 - 3d-4f 340–342
 - 4f 325
 - 5f 342–343
 - formulas and U_{eff} values 343, 344
 - molecular architecture 2
 - in molecular machines 20–23
 - molecular structures 8
 - Mössbauer spectroscopy 174
 - multifunctional 26
 - nitroxide radical 318–321, 331–336
 - $\text{N}_2^{\cdot-}$ radical 336–338
 - nuclear magnetic resonance (NMR) 234, 235

- single-molecule magnets (SMMs) (*contd.*)
- organometallic 15–17
 - polarized neutron diffraction (PND) 235
 - polynuclear complexes 87
 - polynuclear single-molecule magnets 353
 - polynuclear SMMs 143
 - QTM 73–77
 - quantum computing 19–20
 - rational design 17–18
 - recapitulation 167, 169
 - relaxation behaviour 74
 - single-chain magnets (SCMs) 2–4
 - single-ion magnets (SIMs) 4–5
 - single-toroid magnets (STMs) 5–6
 - sulfur-bridged 267
 - synthesis 247
 - thermodynamic properties 89
 - X-ray magnetic circular dichroism (XMCD) 236
- single-toroid magnets (STMs) 5
- mixed-moment 6
 - net toroidal moment 6
- soft bridging groups 267
- Soxhlet extraction 265
- spin contribution 92
- spin Hamiltonian 138–142, 144, 145, 147–169, 178
- spin multiplicity 62, 323
- spin-orbit coupling 4, 11, 12, 14, 96, 97, 103, 136, 209, 231, 246, 272, 283, 284, 286–289, 297, 302, 325, 342, 345
- spin quartet Kramers system 139
- spin triplet non-Kramers species 139
- spin tweaking 258
- square-in-square motif 377
- stable radicals 318
- Star of David topology 378
- stellated cuboctahedron 129
- stepladder manganese(III)
- inverse-[9-MC-3]-metallacrown 108–110
- Stevens operators 101, 139
- stochastic series expansion (SSE)
- quantum Monte Carlo algorithm 115–117
- superparamagnets 9
- synthetic methods
- SIMs
 - 3d-metal 286–289
 - 5f-metal 296–301
 - non-phthalocyanine 4f-metal 291–296
 - phthalocyanine-based 4f-metal 290–291
 - SMMs
 - 3d/4f-metal 273–279
 - 3d/5f-metal 279–281
 - 4f/5f-metal clusters 281–282
 - 4f-metal 262
 - 5f-metal 271–273
 - polynuclear 3d-metal 247
- t**
- [(*talen*^{*t-Bu*}₂)(Mn^{III}(MeOH)₃)₂{Fe^{III}(CN)₆}]³⁺ 233
- [Tb(hfac)₃(NITPhOEt)₂] 333
- [Tb(hfac)₃(NITPhPO(OEt)₂)₂] 336
- [Tb(Pc)(tBu-Pc)] 329
- [Tb(Pc)₂] 326
- [Tb(PcF₆₄)₂]¹⁻ 328
- [Tb(PcF₆₄)₂]²⁻ 328
- [Tb(PcF₆₄)₂]³⁻ 328
- [Tb(picNN)₃] 333
- [Tb(R-Pc)₂] 329
- [Tb{Pc(OEt)₈}₂] 327
- [Tb{Pc(OEt)₈}₂](nBu₄N) 327
- [Tb{Pc(OEt)₈}₂](SbCl₆) 328
- [Tb{Py(OEt)₈}₂][SbCl₆] 290
- [TbPc'₂] 329
- [TbPc'₂]⁺¹ 329
- [TbPc'₂]⁻¹ 329
- 2-(4,4,5,5-tetramethyl-3-oxylimidazole-1-oxide)-5-bromo-3-pyridine 335
- tetra-2-pyridinylpyrazine (tppz) 338
- tetrathiafulvalene (TTF)-based ligands 27
- thermodynamics 45, 47, 48
- 3d-metal carboxylates 250

- 3d metal radical SMMs
 benzosemiquinonoid and nindigo
 radical SMMs 323–325
 carbene radical SMMs 321–323
 nitroxide radical SMMs 318–321
- 3d-metal salt 250
- 3d-metal SIMs synthesis 286–289
- 3d-metal SMMs synthesis
 change of nuclearity 258–262
 end-on (EO) azido group 248
 ferromagnetic exchange interactions
 248
 magnetic exchange coupling 247
 organic ligands 248, 250
 retention of nuclearity 254–258
 single-molecule magnetism 247
 starting materials 250–254
- 3d-4f polynuclear coordination clusters
 (PCCs) 353, 360–362
- Co^{II}-Ln^{III} SMM 368
- Cu^{II}₂Tb^{III}₂ 367
- 1,5M6-1 369
- properties 367
- protonated forms of ligands 371
- rational design 364
- Schiff Base ligands 364, 365, 368
- serendipitous assembly 363, 364
- synthetic approach 363–366
- trinuclear Co^{II}₂Gd complex 368
- trinuclear [Ni^{II}Dy^{III}₂(L7)₆(L15)₄]
 CHCl₃ complex 367
- Zn^{II}₆Ln^{III}₂₄ 363
- Zn^{II}-Ln^{III} complexes 368
- 3d-4f metal radical SMMs 340–342
- 3d/4f-metal SMMs synthesis 273–279
- 3d/5f-metal SMMs synthesis 279–281
- Topological types observed (TTO)
 360
- Topological types of ligands (TTL)
 360
- Topological types of molecules (TTM)
 360
- Topological types of nanoclusters
 (TTN) 360
- Topological types of relations (TTR)
 360
- TOPOS 358, 360
- ToposPro program
 algorithm 361, 362
 analysis steps 361
 completeness 358
 crystallochemical tasks 359
 crystal structures and chemical
 compounds 359
 objectivity 358
 subdivision 358
- ToposPro Topological Collections
 (TTC) 359
- TOPOS topological database (TTD)
 360
- TOPOS topological samples (TTS)
 360
- toroidal magnetic moment 6
- Tp*₂U(2,2'-bpy) 342, 343
- [(TPyA)₂Fe₂(NPhL)](SO₃CF₃) 323
- [(TPyA)₂Fe^{II}₂(NPhL²⁻)]SO₃CF₃)₂ 323
- transuranic SMMs 13
- homoscorpionate complexes 14
- isostructural uranium(III) analogue
 14
- organometallic SMMs 14
- tridentate chelating [Ni(mpko)₃]⁻
 metalloligands 276
- trinuclear Co^{II}₂Gd complex 368
- trinuclear Ni^{II}Dy^{III}₂(L7)₆(L15)₄].CHCl₃
 complex 367
- triphenylmethyl radical 316
- tris(phthalocyaninato)dilanthanide(III)
 SMMs 270
- tunneling 4, 5, 9, 11, 13, 15, 17, 21, 27,
 73, 75–77, 136, 143, 147, 205,
 206, 223, 247, 262, 288, 302, 322,
 329, 332, 366
- U**
- U(III) complex 298
- unquenched orbital angular
 momentum 4, 139, 149, 206,
 213, 246
- [U{H₂B(pz)₂}]₃ 298
- [U{Ph₂B(pz)₂}]₃ 298
- [U(Tp^{Me2})₂I] 298
- [U^{III}₂(μ-C₆H₅CH₃)(HBIPM^{TMS})₂I₂]
 complex 272

$[\{U^V O_2 Ln^{III}(L')(Py)_2\}_2]$ 281
 $[\{U^V O_2(salen)_2 Mn^{II}(Py)_3\}_6]$ cluster
280

Uranium(V) 13, 15, 273, 299, 300

V

variable-temperature
susceptibility 113

verdazyl radicals 317, 340

W

Wigner-Ekharth theorem 89, 107

Wigner 9j symbols 108

X

X-ray magnetic circular dichroism
(XMCD) 4, 236

Z

Zeeman energy 91–93

Zeeman Hamiltonian 179

Zeeman interaction 91, 139

zero adiabatic magnetic susceptibility
53

zero-field splitting (ZFS)

and electronic structure 138

giant-spin approximation 138

giant ZFS 146, 147

and g information extraction

140–143

high-spin systems 136

mononuclear species 138

polynuclear clusters 138

recapitulation 167, 168

rhombic ZFS parameter 165

single-ion ZFS parameter 144

spin-orbit coupling (SOC) 136

spin-spin coupling (SSC) 136

zero-toroidal moment

compounds 6

$Zn^{II}-Ln^{III}$ complexes 368

$Zn^{II}_4 Ln^{III}_2(OH)_2(L44)_2(OAc)_2(NO_3)_2$
(DMF)₃] 375

$[Zn^{II}_5 Ln^{III}(L16)_6(OH)(H_2O)]$ 376