

INDEX

- angular overlap model, 163
- bond lengths, 137, 143, 181, 184, 187, 222
- central-field approximation, 40, 202
- central-field covalency, 200
- chromium(III), 97, 181, 198, 224
 (Cr/Al)₂O₃ – ruby, 214
 Cr(en)₂Br₂⁺, 97, 186
 Cr(en)₂Cl₂⁺, 97, 186
 Cr(en)₂F₂⁺, 97, 186
 Cr(en)₂(H₂O)₂³⁺, 97, 186
 CrF₆³⁻, 126
 Cr(H₂O)₆³⁺, 107
 K₃Cr(CN)₆, 216
- CNDO, 157
- cobalt (II), 198
 Co(imidazole)₆(NO₃)₂, 76
 Co²⁺ in ZnAl₂O₄, 216
 Co(MeCN)₅²⁺, 103
 Co(PhCN)₅²⁺, 103
 CoSiF₆·6H₂O, 75
 Co thiourea₄Cl₂, 102
 Cs₃CoBr₅, 85
 Cs₃CoCl₅, 85
 (Et₄N)₂CoBr₄, 85
 (Et₄N)₂CoCl₄, 85
 (Ph₂MeAsO)₄Co(NO₃)₂, 77, 79
- cobalt(III), 181, 198
 Co(en)₂Cl₂⁺, 102
 CoF₆³⁻, 126
 Co(NH₃)₄Cl₂⁺, 102
 Co(NH₃)₆³⁺, 125, 126
- correlation diagram, 5, 208
- copper(II), 68, 147, 155, 180, 182, 183
 Cs₂CuBr₄, 82, 143, 186
 Cs₂CuCl₄, 82, 143, 144, 147, 186
- Coulomb integrals, 43, 110, 128, 129, 160, 197
- covalency, 113
- crystal spectra
 Cr(en)₂F₂⁺, 97
 Cs₂CuBr₄, 82
 Cs₂CuCl₄, 82
 Cs₂(Mg/Ni)Cl₅, 83
 five-coordinate complexes, 77
 iron (II) octahedral systems, 68
 Nitu₄Cl₂, 102
 (Ph₂MeAsO)₄Co(NO₃)₂, 77
 (Ph₂MeAsO)₄Ni(NO₃)₂, 77
- definitions
 of *B*, 51
 β₃₃, β₃₅, β₅₅, 207, 214
C, 51
Cp, 64, 134
*D*_λ¹, 181
 10*Dq*, 35, 67, 106, 127, 130, 134
Ds, 89, 91
Dt, 89, 91
dσ, 158
dπ, 158
 Δ_{oct}, 35, 67, 127, 130
 Δ_{tet}, 35, 67
*e*_λ, 166
F^{*k*}, 49, 216
*F*_λ³, 165
G^{*l*}, 134
 κ, 90
- diatomic overlap integrals, 196
- differential orbital expansion, 201, 212
- electron correlation, 57
- Eulerian rotations, 167, 181, 189, 191
- exchange integrals, 43, 110, 128, 129, 160, 197
- expansion of 1/*r*_{*ij*}, 32, 43, 48
- expansion theorem, 17
- f*^{*n*} systems, 180, 199
- five-coordinate systems, 77, 80, 103
- ‘frozen core’ method, 123
- Fock operator, 110
- Gaussian orbitals (GTO), 112, 124
- group overlap integrals, 170, 191, 196
- Hartree functions, 51, 109

- Hartree–Fock functions, 51, 109
 ‘hole’ formalisms, 7
 Hückel theory, 160, 161
 Hund’s formula, 1
 hybrid orbitals, 8, 142
 hydrogenic wavefunctions, 107, 151, 153
- inhomogeneous orbital expansion, 221, 225
- interelectron repulsion parameters, 48, 197, 202, 203
- iron(II), 67, 98, 198
 FeF_6^{4-} , 126
 Fe isoquinoline₄Br₂, 99
 Fe isoquinoline₄Cl₂, 99
 Fe isoquinoline₄I₂, 99
 Fe γ -picoline₄X₂ (X = Cl, Br, I), 101
 Fepy₄Br₂, 99, 101
 Fepy₄Cl₂, 99, 101
 FeSiF₆·6H₂O, 68, 74
 FeSO₄·(NH₄)₂SO₄·12H₂O, 68, 74
 Fe thiourea₄Cl₂, 102
- iron(III), 8, 9, 198
 FeF_6^{3-} , 9, 122, 126
 $\text{Fe}(\text{CN})_6^{3-}$, 8
- Legendre polynomials, 44
- magnetic anisotropy
 origin of, 3
 Co(imidazole)₆(NO₃)₂, 76
 Co thiourea₄Cl₂, 102
 CoSiF₆·6H₂O, 75
 Cs₃CoBr₅, 85
 Cs₃CoCl₅, 85
 (Et₄N)₂CoBr₄, 85
 (Et₄N)₂CoCl₄, 85
 (Et₄N)₂NiCl₄, 87
 FeSiF₆·6H₂O, 74
 FeSO₄·(NH₄)₂SO₄·12H₂O, 74
 Fe thiourea₄Cl₂, 102
 Mn thiourea₄Cl₂, 102
 Ni thiourea₄Cl₂, 102
 (Ph₂MeAsO)₄Co(NO₃)₂, 79
 (Ph₂MeAsO)₄Ni(NO₃)₂, 79
- manganese(II), 198
 MnF₂, 11
 MnF_6^{4-} , 122, 126
 $\text{Mn}(\text{H}_2\text{O})_6^{2+}$, 11
- many-electron systems, 39, 124
 McClure’s model, 98, 158
 molecular orbitals, 11, 109
 Mössbauer results, 101
 multipole expansions, 32, 48
- Nephelauxetic Series, 198
- nickel(II), 2, 37, 83, 183, 198
 $\text{Ni}(\text{en})_2(\text{H}_2\text{O})_2^{2+}$, 102
 NiF_6^{4-} , 113, 114, 121, 123, 126
 Ni(NH₃)₄(NCS)₂, 158
 Ni(*N,N*-dimethyl-en)₂(H₂O)₂²⁺, 102
 Nipy₄Br₂, 94, 186
 Nipy₄Cl₂, 94, 144, 186
 Ni pyrazole₄Br₂, 186
 Ni pyrazole₄Cl₂, 96, 144, 186
 Ni thiourea₄Cl₂, 102
 Cs₃(Mg/Ni)Cl₅, 83, 144, 147
 (Et₄N)₂NiCl₄, 87
 (Ph₂MeAsO)₄Ni(NO₃)₂, 79
- non-crossing rule, 6
- orbital quenching, 2
 orbit–orbit interaction, 56
- point-charge model, 31, 134, 151
 point-dipole calculations, 151
 polarization correction, 54
- resonance integral, 161
 restricted Hartree–Fock (RHF) method, 111, 119
 Roothaan equations, 111
- semi-empirical MO methods, 15, 157
 Slater determinants, 41
 Slater’s rules, 153
 Slater orbitals (STO), 109
 Spectrochemical Series, 10, 97, 101, 199
- spectral results (*see also* crystal spectra)
 $\text{Co}(\text{en})_2\text{Cl}_2^+$, 102
 $\text{Co}(\text{MeCN})_5^{2+}$, 103
 $\text{Co}(\text{NH}_3)_4\text{Cl}_2^+$, 102
 $\text{Co}(\text{PhCN})_5^{2+}$, 103
 $\text{Cr}(\text{en})_2\text{Br}_2^+$, 97
 $\text{Cr}(\text{en})_2\text{Cl}_2^+$, 97
 $\text{Cr}(\text{en})_2(\text{H}_2\text{O})_2^{3+}$, 97
 Fe isoquinoline₄X₂ (X = halogen), 99

Index

235

- Fe γ -picoline₄X₂ (X = halogen), 101
 Fe₄Br₂, 99
 Fe₄Cl₂, 99
 iron(II) octahedral systems, 11
 MnF₂, 11
 Mn(H₂O)₆²⁺, 11
 Ni(en)₂(H₂O)₂²⁺, 102
 Ni(*N,N*-dimethyl-en)₂(H₂O)₃²⁺, 102
 Nipy₄Br₂, 94
 Ni pyrazole₄Cl₂, 96
 spin-only formula, 2
 steric hindrance, 101
 sum rules, 176
 symmetry-restricted covalency, 200
 titanium(III)
 TiF₆³⁻, 126
 Trees' correction, 54
 unrestricted Hartree-Fock (UHF) method, 111, 119
 valence bond method, 123
 Van Vleck's formula, 2
 vector triangle rule, 23
 VSIE, 162
 VOIP, 162
 Wolfsberg-Helmholz model, 157, 162
 ZDO, 157
 zeta functions, 112