

---

## Author Index Volumes 101–106

- Aldinger F, see Seifert HJ (2002) *101*: 1–58  
Amstutz N, see Hauser A (2003) *106*: 81–96  
Anitha S, Rao KSJ (2003) The Complexity of Aluminium-DANN Interactions: Relevance to Alzheimer's and Other Neurological Diseases. *104*: 79–98  
Aramburu JA, see Moreno M (2003) *106*: 127–152  
Atanasov M, Daul CA, Rauzy C (2003) A DFT Based Ligand Field Theory *106*: 97–125  
Atwood DA, see Conley B (2003) *104*: 181–193  
Atwood DA, Hutchison AR, Zhang Y (2003) Compounds Containing Five-Coordinate Group 13 Elements. *105*: 167–201
- Barriuso MT, see Moreno M (2003) *106*: 127–152  
Bellandi F, see Contreras RR (2003) *106*: 71–79  
Berend K, van der Voet GB, de Wolff FA (2003) Acute Aluminium Intoxication. *104*: 1–58  
Bohrer D, see Schetinger MRC (2003) *104*: 99–138  
Bowlby BE, Di Bartolo B (2003) Spectroscopy of Trivalent Praseodymium in Barium Yttrium Fluoride *106*: 191–208  
Budzelaar PHM, Talarico G (2003) Insertion and  $\beta$ -Hydrogen Transfer at Aluminium. *105*: 141–165
- Cancines P, see Contreras RR (2003) *106*: 71–79  
Conley B, Atwood DA (2003) Fluoroaluminates Chemistry. *104*: 181–193  
Contreras RR, Suárez T, Reyes M, Bellandi F, Cancines P, Moreno J, Shahgholi M, Di Bilio AJ, Gray HB, Fontal B (2003) Electronic Structures and Reduction Potentials of Cu(II) Complexes of [N,N'-alkyl-bis(ethyl-2-amino-1-cyclopentenecarbothioate)] (alkyl = ethyl, propyl, and butyl) *106*: 71–79
- Daul CA, see Atanasov M (2003) *106*: 97–125  
Day P (2003) Whereof Man Cannot Speak: Some Scientific Vocabulary of Michael Faraday and Klixbüll Jørgensen *106*: 7–18  
Delahaye S, see Hauser A (2003) *106*: 81–96  
Di Bartolo B, see Bowlby BE (2003) *106*: 191–208  
Di Bilio AJ, see Contreras RR (2003) *106*: 71–79
- Fontal B, see Contreras RR (2003) *106*: 71–79  
Frenking G, see Lein M (2003) *106*: 181–191  
Frühauf S, see Roewer G (2002) *101*: 59–136  
Frunzke J, see Lein M (2003) *106*: 181–191
- Gray HB, see Contreras RR (2003) *106*: 71–79  
Güdel HU, see Wenger OS (2003) *106*: 59–70
- Haubner R, Wilhelm M, Weissenbacher R, Lux B (2002) Boron Nitrides – Properties, Synthesis and Applications. *102*: 1–46

- Hauser A, Amstutz N, Delahaye S, Sadki A, Schenker S, Sieber R, Zerara M (2003) Fine Tuning the Electronic Properties of  $[M(\text{bpy})_3]^{2+}$  Complexes by Chemical Pressure ( $M = \text{Fe}^{2+}, \text{Ru}^{2+}, \text{Co}^{2+}$ , bpy = 2,2'-bipyridine) *106*: 81–96
- Herrmann M, see Petzow G (2002) *102*: 47–166
- Herzog U, see Roewer G (2002) *101*: 59–136
- Hoggard PE (2003) Angular Overlap Model Parameters *106*: 37–57
- Höpfel H (2002) Structure and Bonding in Boron Containing Macrocycles and Cages. *103*: 1–56
- Hutchison AR, see Atwood DA (2003) *105*: 167–201
- Jansen M, Jäschke B, Jäschke T (2002) Amorphous Multinary Ceramics in the Si-B-N-C System. *101*: 137–192
- Jäschke B, see Jansen M (2002) *101*: 137–192
- Jäschke T, see Jansen M (2002) *101*: 137–192
- Jaworska M, Macyk W, Stasicka Z (2003) Structure, Spectroscopy and Photochemistry of the  $[M(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2]_2$  Complexes ( $M = \text{Fe}, \text{Ru}$ ) *106*: 153–172
- Lein M, Frunzke J, Frenking G (2003) Christian Klíxbüll Jørgensen and the Nature of the Chemical Bond in  $\text{HArF}^{\dagger}$  *106*: 181–191
- Linton DJ, Wheatley AEH (2003) The Synthesis and Structural Properties of Aluminium Oxide, Hydroxide and Organooxide Compounds. *105*: 67–139
- Lux B, see Haubner R (2002) *102*: 1–46
- Macyk W, see Jaworska M (2003) *106*: 153–172
- Mahalakshmi L, Stalke D (2002) The  $\text{R}_2\text{M}^+$  Group 13 Organometallic Fragment Chelated by P-centered Ligands. *103*: 85–116
- Moreno J, see Contreras RR (2003) *106*: 71–79
- Moreno M, Aramburu JA, Barriuso MT (2003) Electronic Properties and Bonding in Transition Metal Complexes: Influence of Pressure *106*: 127–152
- Morsch VM, see Schetinger MRC (2003) *104*: 99–138
- Mossin S, Weihe H (2003) Average One-Center Two-Electron Exchange Integrals and Exchange Interactions *106*: 173–180
- Müller E, see Roewer G (2002) *101*: 59–136
- Oshiro S (2003) A New Effect of Aluminium on Iron Metabolism in Mammalian Cells. *104*: 59–78
- Patočka J, see Strunecká A (2003) *104*: 139–180
- Petzow G, Herrmann M (2002) Silicon Nitride Ceramics. *102*: 47–166
- Power P (2002) Multiple Bonding Between Heavier Group 13 Elements. *103*: 57–84
- Rao KSJ, see Anitha S (2003) *104*: 79–98
- Rauzy C, see Atanasov (2003) *106*: 97–125
- Reisfeld R (2003) Rare Earth Ions, Their Spectroscopy of Cryptates and Related Complexes in Glasses *106*: 209–237
- Reyes M, see Contreras RR (2003) *106*: 71–79
- Roewer G, Herzog U, Trommer K, Müller E, Frühauf S (2002) Silicon Carbide – A Survey of Synthetic Approaches, Properties and Applications. *101*: 59–136
- Sadki A, see Hauser A (2003) *106*: 81–96
- Schäffer CE (2003) Axel Christian Klíxbüll Jørgensen (1931–2001) *106*: 1–5
- Schenker S, see Hauser A (2003) *106*: 81–96
- Schetinger MRC, Morsch VM, Bohrer D (2003) Aluminium: Interaction with Nucleotides and Nucleotidases and Analytical Aspects of Determination. *104*: 99–138
- Schmidtke HH (2003) The Variation of Slater-Condon Parameters  $F^k$  and Racah Parameters B and C with Chemical Bonding in Transition Group Complexes *106*: 19–35

- Schubert DM (2003) Borates in Industrial Use. *105*: 1–40
- Schulz S (2002) Synthesis, Structure and Reactivity of Group 13/15 Compounds Containing the Heavier Elements of Group 15, Sb and Bi *103*: 117–166
- Seifert HJ, Aldinger F (2002) Phase Equilibria in the Si-B-C-N System. *101*: 1–58
- Shahgholi M, see Contreras RR (2003) *106*: 71–79
- Sieber R, see Hauser A (2003) *106*: 81–96
- Stalke D, see Mahalakshmi L (2002) *103*: 85–116
- Stasicka Z, see Jaworska M (2003) *106*: 153–172
- Strunecká A, Patocka J (2003) Aluminofluoride Complexes in the Etiology of Alzheimer's Disease. *104*: 139–180
- Suárez T, see Contreras RR (2003) *106*: 71–79
- Talarico G, see Budzelaar PHM (2003) *105*: 141–165
- Trommer K, see Roewer G (2002) *101*: 59–136
- Uhl W (2003) Aluminium and Gallium Hydrazides. *105*: 41–66
- van der Voet GB, see Berend K (2003) *104*: 1–58
- Weihe H, see Mossin S (2003) *106*: 173–180
- Weissenbacher R, see Haubner R (2002) *102*: 1–46
- Wenger OS, Güdel HU (2003) Influence of Crystal Field Parameters on Near-Infrared to Visible Photon Upconversion in  $\text{Ti}^{2+}$  and  $\text{Ni}^{2+}$  Doped Halide Lattices *106*: 59–70
- Wheatley AEH, see Linton DJ (2003) *105*: 67–139
- Wilhelm M, see Haubner R (2002) *102*: 1–46
- de Wolff FA, see Berend K (2003) *104*: 1–58
- Zerara M, see Hauser A (2003) *106*: 81–96
- Zhang Y, see Atwood DA (2003) *105*: 167–201

---

# Subject Index

- Absorption bands, shapes 2  
Absorption measurements 195  
Absorption spectra 2, 3, 30  
Acetic acid 220  
Acidic catalyst 214, 215  
Activation energy 89, 94  
Alcohol solvation 1  
Alumina 213  
Amine 239  
Amorphous phases 215  
Anderson theory 173  
Angular overlap model (AOM) 3, 20, 25, 29–33, 99, 177, 249  
Antenna effect 210  
Antibonding, 10Dq 147  
AOM *see* Angular overlap model  
AOM matrix elements 42  
AOM parameter values, amine assumption 43, 50, 55  
– – –, amines 43, 48  
– – –, carboxylates 48  
– – –, cyanide 48, 49  
– – –, photochemical reactivity 52  
– – –, thermal reactivity 54  
– – –, *trans* effect 54  
– – –, transferability 42, 49, 56  
– – –, uncertainties 46, 48  
AOM parameters 177  
AOMX 110  
Argon-fluorine interactions 181, 188  
Average of configuration (AOC) 108  
  
Barium yttrium fluoride (BaY<sub>2</sub>F<sub>8</sub>) 193–195  
BaY<sub>2</sub>F<sub>8</sub>:Pr<sup>3+</sup> 197–203  
Bio-inorganic chemistry 99  
2,2'-Bipyridine 227  
Bis(carbonylcyclopentadienyliron) 153, 154, 160, 167  
Bis(dicarbonylcyclopentadienylmetallate) 154  
Bis(dicarbonylcyclopentadienylosmium) 155  
  
Bis(dicarbonylcyclopentadienylruthenium) 153, 154, 165, 168  
Blue copper protein 79  
Blue shift, pressure, TM complexes 139  
Born-Oppenheimer approximation 227  
Bromides 65  
  
Candoluminescence 251  
Carbonyl compounds 153  
Carboxydithioc acid 73  
Cellular ligand field 20  
CERI *see also* Cyanamid European Research Institute  
CF model 129  
CFT 99  
C-H bond activation 169  
Charge transfer 227, 230  
Charge transfer absorption 248  
Charge transfer spectra 4  
Charge transfer states 65  
– – –, electronic relaxation 140  
Charge transfer transitions 127  
– – –, pressure influence 137  
Charge, effective 23  
Chlorides 65  
Chlorobenzene 218  
Chromophores 244  
–, orthoaxial 38  
CI 105  
CI-DFT 98, 122  
CILF program 97  
Cobalt(III) 249  
Concentration quenching 226  
Condensation reaction 214  
Configuration, electron 21–24  
Conformers 155  
Cooperative effects 94  
Copper(II) 244  
Corrections, second-order 105  
Coulomb integral 23  
Covalency 4, 59, 66  
–, central-field 21, 26

- Cr(III) dimers, oxo-bridged 174  
Crystal field (CF) 60, 61, 66, 129, 212  
Crystal field theory (CFT) 3, 99  
CT manifold/energies 176  
CT transitions 127, 144  
– –, pressure influence 137  
Cu(II) complexes 71, 72, 74, 78  
Cu(II)/Cu(I) reduction potentials 72  
Cu<sup>2+</sup> complexes, tetragonal 143  
CuN<sub>2</sub>S<sub>2</sub> coordination 71, 75  
CuX<sub>4</sub>Y<sub>2</sub> complex, metal-ligand distance, pressure 144  
Cyanamid European Research Institute 4, 237, 241–249  
Cyclopentadienyl compounds 153  
Cyclopentanone 73
- d-d absorption** 65  
– spectra 72  
– transitions, optical 99  
Denmark, Technical University 1  
–, University of Copenhagen 4  
Density functional theory (DFT) 138  
– – –, time-dependent 98  
DFT calculation, bis(carbonylcyclopentadienyliron) 153  
– –, bis(dicarbonylcyclopentadienyl-ruthenium) 153  
– –, electronic spectra 159  
– –, molecular orbitals 159  
– –, molecular structure 155  
Diamagnetism 10  
Dip-coating 213, 220  
Dipole-dipole contribution 229  
Di-urethane-siloxane (DURS) 216–219  
Donor-acceptor bonds 184  
Dry gel 214  
Dyes, organic 213  
Dynamic coupling mechanism 226  
Dynamic luminescence 221
- Electric dipole 211, 212, 221, 228, 229  
Electrode 9  
Electroluminescence device 211  
Electrolyte 9  
Electromagnetism 8  
Electron affinity 244  
– localization 131  
– transfer spectra 4  
Electron-electron repulsion 20, 23, 26  
Electronic charge 225  
Electronic ground state 20  
Electronic spectra 20, 21, 32, 34, 77  
– –, bis(carbonylcyclopentadienyliron) 160  
– –, bis(carbonylcyclopentadienylruthenium) 165  
– –, DFT calculation 159  
Electronic spin resonance (ESR) 99  
Electronic transition 22, 23  
Electrostatic model 3  
Electrostatic point charge approximation theory 212  
Elements, superheavy 252  
Emission quantum yield 228  
Emitting level 227, 233  
Encapsulated ion 229, 233  
Energy levels 20  
Energy matrix elements 30  
Energy transfer 227–230  
Epoxy polymerization 216, 218  
Epoxy-silica-ormosil (ESOR) 216–218  
EPR 109  
– spectra 71, 75, 76  
Error, mean square 30  
Europium cryptate 220, 221, 230, 233  
Europium(III) 245  
Exchange interactions 173  
Excited states 98  
– –, metastable 60, 64, 69
- Faraday, M. 8  
Fermi's golden rule 227  
Fluoroprovskites 131  
Forced electric dipole mechanism 226  
Frank-Condon energy/factors 90, 228  
Free ion 22, 27–33  
FTIR spectral data 75
- Gap energy 226  
Geneva, University 4, 242, 252  
Germanate 213  
Glass ceramics, translucent 248  
Glasses 210–215  
Glycid oxypropyl trimethoxysilane (GLYMO) 216, 218, 230  
Goodenough-Kanamori rules 173  
Griffith's parameter 101, 109  
Ground state 98  
– – manifold 176
- HArF** 181  
–, electronic structure 184  
–, energy partitioning analysis 187  
Heisenberg-Dirac-van Vleck exchange parameter 173  
Helium compounds 182  
Hellmann-Feynman theorem 24  
High-spin 32  
Hydrofluoric acid 214

- Hydrogen function 23  
Hydrogen-argon interactions 181  
Hydrolysis reaction 213, 214  
Hydroxyl ion 214  
Hypersensitive transition 213  
Hypersensitivity 241, 242
- Insulators, transition metal impurities 130  
Interelectronic repulsion parameters 21, 26, 30, 32, 103  
Intersystem crossing 84  
Ionic colours 12  
IR spectra 74  
Iridium(III) 242, 243, 249  
Iron, bis(carbonylcyclopentadienyliron) 160  
Isocyanatopropyl triethoxysilane (ISTEOS) 217, 219
- Janack's theorem 107  
Jørgensen rule, ligand substitution 141  
Jørgensen spin-pairing energy parameter 174  
Judd-Ofelt intensity parameters 228  
Judd-Ofelt theory 198
- Kasha's rule 60  
Klixbüll, J. 10, 38–40, 43, 55, 56  
Kohn-Sham orbitals 101, 105  
Kronecker delta function 226
- Lanthanide compounds 221  
Lanthanide ions, electronic states 228  
Laporte rule 210  
Least square fitting 105  
LFDFT, hybrid 109, 113  
Lifetime measurements 197  
Ligand field 3, 5, 20, 25, 29–33, 81–83, 97  
– – hamiltonian 99  
– – states 83  
– – strength 81, 83  
– – theory 5, 20, 25, 29–33, 97  
– – treatment 3  
Ligands, geometrical arrangement 128  
–, innocent 13  
Light conversion molecular device 210, 211  
Liquids 213  
Low-phonon host 60  
Luminescence 86  
– measurements 196  
Luminescence probes, biomedical assays 211
- Magnetic dipole strength 225  
Magnetic interactions/properties 98, 99
- Manganese(III) dimers, oxo-bridged 174  
Matlab 107  
Matrix materials 215–219, 230  
– –, undoped 234  
MCD 109  
Metal-ligand distance, 10Dq 147  
– –, dependence 136  
– –, pressure 129, 130  
– –, variations 127  
Metal-to-ligand charge transfer (MLCT) 83, 86  
2-Methoxyethanol 220  
Microcrystalline parameters 212  
ML<sub>6</sub> complex, ground state 134  
Mn(III) dimers, oxo-bridged 174  
Mn<sup>2+</sup> impurities, KMgF<sub>3</sub> 132  
MO coefficients 108  
Molar ratio 218–220  
Molecular orbitals 20–23  
Molecular structure, bis(carbonylcyclopentadienyliron) 154  
– –, bis(carbonylcyclopentadienylruthenium) 154  
– –, DFT calculation 155  
Molecular symmetry 20, 30  
Multiphonon emission 226  
– relaxation 64, 84  
Multiplet energies 113  
– splitting 103  
Multipolar interactions 229
- NATO Science Adviser's Office 4  
Neodymium 241  
Nephelauxetic effect 12, 21, 26, 29, 213, 246  
– quotient 22, 32  
– series 3, 34, 81  
Noble gas chemistry 183  
– – compounds 181, 183  
Noncentrosymmetric interactions 211  
Nonexponential decay 226  
Nonradiative decay mechanism 226  
– processes 87  
– relaxation 61, 67, 84, 227, 233  
– transition probabilities 226, 227  
Nucleophilic reagents 219
- One-center two-electron exchange integral 173  
Optical electronegativity 246  
Optical process, nonlinear 60  
Optical properties 98  
Optimization procedure 30  
Orbital energies 20  
Organometallic compounds 215

- Organosilicate glass 215  
Ormocer hybrid material 216  
Osmium, bis(dicarbonylcyclopentadienylosmium) 155  
Oxalate network 86, 90, 91  
Oxidation numbers 14  
Oxidation states 14
- Paramagnetism 10, 99  
Pentammine effect 2  
Phase-coupling 20  
Phlogiston 243  
Phonons, Raman scattering 203  
–, virtual 206  
Photochemistry, bis(dicarbonylcyclopentadienyliron) 167  
–, bis(dicarbonylcyclopentadienylruthenium) 168  
Photoelectron spectroscopy 248, 251  
Planck's constant 225  
Plutonium(III) 239  
Point-charge formalism 2  
Point-dipole formalism 2  
Polyethylene glycol (PEG) 216–219  
Praseodymium 193, 194  
Preponderant configuration 12  
Pressure, chemical, metal-ligand distances 129, 130  
*n*-Propanol 220  
Pulsed excitation data 201
- Quanticle 14  
Quantum efficiency 226  
Quantum mechanical model 20  
Quantum paradoxes 244  
Quarkonium chemistry 246, 252  
Quarks, chemistry 4  
Quasi-resonance conditions 229
- Racah parameters 65, 100, 129, 241  
– – changes 29, 32, 33  
Random strains 143  
Rare earth complexes 31  
Reduction factors 21  
Reduction potentials 77  
Reflectance spectra 30  
Refractive index 212, 216  
Relaxation, high/low-spin 84, 85  
–, multiphonon 64, 84  
–, – emission 226  
–, nonradiative 61, 67, 84  
Rhodium(III) 249  
Ruthenium, bis(dicarbonylcyclopentadienylruthenium) 153, 154, 165, 168  
–, hydride 169
- Samarium(III) 239  
SCCEH calculations 136  
Semiempirical method 20, 25, 34  
Sequestrating agent 211  
Silane, isocyanate functionalized 218  
Silanol 214, 215  
Silica glass 211  
Silicates 213–215  
–, organically modified (Ormosils) 213, 215  
Silicon alkoxide 213  
Silicon hybrids 211  
Slater determinants 97  
Slater function 23  
Slater-Condon parameters 100  
Sol particles 214  
Solar collectors, luminescent 248  
Sol-gel glasses 244, 248  
Sol-gel process 211–214, 233  
Solvation effect 239  
Solvay Conference/Report 3  
Spectral lines, thermal effects 203  
Spectrochemical series 81  
Spin multiplicity 2  
Spin transition 92  
Spin-coating 213  
Spin-crossover 82, 83  
Spin-forbidden transitions 2  
Spin-orbit coupling 30–32, 109  
Spin-pairing energy 173  
Stevens delocalization coefficients 21  
Sulfide ion 220, 221
- Taxology 15  
Terbium sulfide 219, 221, 231, 233  
Tetraalkoxysilane (TAOS) 213  
Tetraethoxysilane (TEOS) 213, 214  
Tetramethoxysilane (TMOS) 213, 218  
Thermalization 201  
Thiocyanate 221  
Time-dependent DFT 98  
Time-resolved spectra 201  
Titania 213  
TM complexes 97, 127, 227  
– –, molybdates 227  
– –, octahedral 133  
– –, tungstate/vanadates 213, 227  
TM impurities, electronic properties 130  
Transferred electronic state, pressure dependence 145  
Transition metal (TM) complexes 97, 127  
Transition probabilities 212, 227, 230  
Transparent coatings 215  
Trees correction 30  
Triplet state 229  
Trivalent logic 4

- trans*-Uranium elements 4  
Uranyl photophysics 248  
Urethane 216,218  
UV dosimeters 211  
UV-VIS spectra 76,239
- Valency, misdirected 20  
van der Waals complex 184  
Vibronic lines 198
- Wavefunction 24,25,27  
-, symmetry-adapted 103
- Wet gel 214  
Wigner-Eckhart's theorem 100  
Wolfberg-Helmholz guess 146
- X-ray photoelectron spectroscopy 4  
Xerogel 214
- Zero-point energy difference 84,90,92  
Zirconia 213  
- /GLYMO 219,220  
Zirconium oxide 216-219  
Zirconium-*n*-tetrapropoxide 218,220