#### а

α-rhombohedral boron 139-140 metal position in periodic system β-effect 371-372 284 - 286β-rhombohedral boron 140–142 - adsorbate coordination in relation to  $\pi$ -bonding. *See* heavy main-group atoms adsorbate valence 301-303 multiple bonding - molecular adsorption and CO adsorption  $\pi$  helix. See 3<sub>10</sub> helix 286-296  $\pi$ -conjugation in donor-substituted - surface group orbitals 296-301 adsorbate bond activation and formation cyanoethynylethenes 365-366 - different metal surfaces reactivity 317,  $\pi$ -conjugation in tunable bis(gem-diethynylethene) fluorophores 318-321 quantum-chemical view of bond activation 366, 368, 369 321 - 328σ-hole 525, 526, 528, 531 adsorbate coordination in relation to adsorbate 2p shell accounts radial nodes lack 2-4 valence 301-303 - high electronegativity and small size of alkali metal clusters 172 2p-elements 4-7 alkali metal-indium clusters 142-143 - hybridization defects influence on magnetic alloying 303-305 resonance parameters 14-15 anisotropy of current (induced) density - inert-pair effect and dependence on partial (ACID) 396-403, 404 charge of central atom 7-10 anisotropy of magnetic susceptibility and - multiple-bond paradigm and bond strengths exaltation 387-391 13 - 14annulene 390, 395, 401, 402, 409 - stereo-chemically active versus inactive lone aromatic compounds and transition states pairs 10-12 magnetic properties 383-384 310 helix 506 examples 4n+2 interstitial electron rule and ring-cap – aromatic transition states 406, 407–411 orbital overlap compatibility 122-125 – – benzene and borazine 397–398 *ab initio* and density functional theory – – coarctate transition states 411, 413–415 calculations of water dimer 510 -- fullerenes 400-401 actinocene 351 -- homoaromatic molecules 403-405 actinyls 349-350 -- Hückel and Möbius structures 401-403 active spaces 253-255, 265 -- organometallic compounds 404, 406 adaptive natural density partitioning (AdNDP) - - pyridine, phosphabenzene, and 425-426, 429, 433, 438, 439 silabenzene 398-399 adatom adsorption energy dependence on - molecules magnetic properties 386-387 coordinative unsaturation of surface atoms – anisotropy of magnetic susceptibility and 276 - 283exaltation 387-391

*The Chemical Bond: Chemical Bonding Across the Periodic Table,* First Edition. Edited by Gernot Frenking, Sason Shaik.

© 2014 Wiley-VCH Verlag GmbH & Co. KGaA. Published 2014 by Wiley-VCH Verlag GmbH & Co. KGaA.

- adatom adsorption energy as function of

```
aromatic compounds and transition states
    magnetic properties (contd.)
-- chemical shifts in NMR 391-392
-- quantum theoretical treatment 392-397
aromaticity 372-784. See also inorganic
  aromatic compounds
- historical review 384-386

    in group 14 cyclopropenylium cation

    homologs 375-376
- in metallabenzenes 376-378
- in neutral exocyclic substituted
    cyclopropenes (HC)<sub>2</sub> C=X 374-375
Aromatic Ring-Current Sheildings method
  (ARCS) 424
aromatic stabilization energies (ASEs) 358,
  359
atoms in molecules (AIM) 237-238
```

### b

Ba<sub>7</sub>Ga<sub>4</sub>Sb<sub>9</sub> 470-473 band structures 449 Becke-Johnson (BJ) damping 489 benzene and borazine 397-398 Bloch orbitals 447-449 block-localized wavefunction (BLW) 515 blueshifting hydrogen bonds 516 bond activation quantum-chemical view - (100) surface uniqueness 323-325 - molecular  $\pi$  bond activation (particle shape dependence) 321-323 - molecular  $\pi$  bond activation 325-328 bond order overlap population (BOOP) 275 bond orders analysis 235-237 Born-Oppenheimer approximation 524 Born-von Karman periodic boundary conditions 447 Brillouin zone 449 broken spin symmetry 233-235 Brønsted-Evans-Polanyi relation 317, 320, 321, 325, 330, 333

#### С

capping principle 125-126 carbones 73-81 carbonyl complexes 181-187 coarctate transition states 411, 413-415 complete-active-space configuration-interaction (CASCI) 227 complete-active-space self-consistent-field (CASSCF) approach 225-227, 245, 348, 349, 351, 352 complete-graph tensor-network (CGTN) 228-229

condensed polyhedral clusters stability affecting factors - exo-polyhedral interactions 134-135 - orbital compatibility 135-136 configuration interaction ansatz 222 - density matrices 222-223 - truncation procedure 222 conjugation - correlation with experimental data - in 1,3-butadienes, 12.1,3-butadiyne, polyenes, and enones 361-363  $- - \pi$ -conjugation in donor-substituted cyanoethynylethenes 365-366  $- - \pi$ -conjugation in tunable bis(gem-diethynylethene) fluorophores 366, 368, 369 -- Hammett and Hammett-Brown substituent constants 363-365 Coulomb interaction 523, 524, 526, 528-530, 533 Coulomb repulsion overcoming in transition metal complex 494-495 covalency and actinides 342-347 covalent bonds in polar metallic solids 459-462 Cr, Mo, and W<sub>2</sub> containing complexes 259-263 crystal orbital Hamilton population (COHP) 455, 468, 470 crystal orbital overlap population (COOP) curves 455, 468 crystal orbitals 449 crystal versus electronic structure 466-470

# d

democracy principle 67 density functional theory (DFT) 229-230, 276, 277, 284, 286, 288-289, 302, 306, 307, 322, 326, 446, 447, 455, 461, 463, 464-465, 482, 510-511 density-matrix renormalization group (DMRG) algorithm 227-228, 240, 241, 242, 245, 246 density of states (DOS) 461, 463, 471, 472 - analysis 453-456 Dewar-Chatt-Duncanson (DCD) model 176 diabatic states model 66-67 diamagnetism 387 diatomic molecules bonding analysis 27-29 Diels-Alder reaction 406, 408, 409 difference-density techniques 531-533 different metal surfaces reactivity 317, 318-321 directional electrostatic bonding 523-524

 anisotropic molecular electrostatic potential distribution around atoms 524-528 - difference-density techniques 531-533 - directional noncovalent interactions 533 electrostatic anisotropy, donor-acceptor interactions and polarization 528-530 purely electrostatic models 530–531 directional noncovalent interactions 533 dispersion correction 486, 488-490, 492-493, 495 dispersion interaction 477-480 examples - - Coulomb repulsion overcoming in transition metal complex 494-495 – hexamethylethane derivatives 493–494 -- substituted ethenes 492-493 - London dispersion energy theory 480-485 - theoretical methods to compute dispersion energy 485 – – general 486 – supermolecular density functional theory 488-490 – supermolecular wave function theory (WFT) 486-488 - - symmetry-adapted perturbation theory (SAPT) 490, 491 donor-acceptor bonding 175, 176, 188, 190, 192, 193, 195, 196, 203, 207, 211 donor-acceptor complexes of main-group elements 71-73 - EL<sub>2</sub> single-center 73 – – CL<sub>2</sub> carbones 73–81 – donor–acceptor bonding in heavier tetrylenes ER2 and tetrylones EL2 (E=Si-Pb) 88-94 – isoelectronic group 15 and group 13 homologues (N<sup>+</sup>)L<sub>2</sub> and (BH)L<sub>2</sub> 82 - 88 – E<sub>2</sub>L<sub>2</sub> two-center complexes 94–95 -- Si<sub>2</sub>L<sub>2</sub>-Pb<sub>2</sub>L<sub>2</sub> (L=NHC) 95-101 - - two-center group 13 and group 15 complexes B<sub>2</sub>L<sub>2</sub> and N<sub>2</sub>L<sub>2</sub> 101-110 donor-acceptor interactions 28, 36, 37, 38, 40, 41, 44-46. See also dispersion interaction double bonding 13, 15, 16 EL<sub>2</sub> single-center 73

 CL<sub>2</sub> single center 73–81
 CL<sub>2</sub> carbones 73–81
 donor-acceptor bonding in heavier tetrylenes ER<sub>2</sub> and tetrylones EL<sub>2</sub> (E=Si-Pb) 88–94
 isoelectronic group 15 and group 13

E<sub>2</sub>L<sub>2</sub> two-center complexes 94–95 - Si<sub>2</sub>L<sub>2</sub>-Pb<sub>2</sub>L<sub>2</sub> (L=NHC) 95-101 - two-center group 13 and group 15 complexes B<sub>2</sub>L<sub>2</sub> and N<sub>2</sub>L<sub>2</sub> 101-110 electron correlation 254, 266, 480, 482, 486, 495, 496 -- effects 224, 225, 227, 239, 240, 242, 245 electron-counting rules in cluster bonding 113-114 - 4n+2 interstitial electron rule and ring-cap orbital overlap compatibility 122-125 - capping principle 125-126 - electronic requirement of condensed polyhedral boranes and mno rule 126-134 electronic structure of elemental boron and boron-rich metal borides 139  $- - \alpha$ -rhombohedral boron 139–140  $--\beta$ -rhombohedral boron 140–142 – alkali metal-indium clusters 142–143  $- - Mg_{\sim 5}B_{44}$  electronic structure 143–144 - factors affecting stability of condensed polyhedral clusters -- exo-polyhedral interactions 134-135 -- orbital compatibility 135-136 - hypoelectronic metalloboranes 136-138 - localized bonding schemes for bonding in polyhedral boranes 119-122 - Wade's rules 114-119 electron density distribution analysis 513-514 electronic localization 456-458, 462-466 electron localization function (ELF) 456.514 - f block applications 341-342 - magnetic versus metallic behavior in K<sub>4</sub> P<sub>3</sub> 462-466 electrostatic and orbital interactions 509 - 510electrostatic anisotropy, donor-acceptor interactions and polarization 528-530 elemental boron and boron-rich metal borides electronic structure 139 – α-rhombohedral boron 139–140  $-\beta$ -rhombohedral boron 140–142 - alkali metal-indium clusters 142-143

– Mg<sub>~5</sub>B<sub>44</sub> electronic structure 143–144

```
energy decomposition analysis (EDA) 181,
  182, 185, 188, 191, 193, 194, 197, 202, 207,
  359-360, 373, 374, 376, 378, 482, 483, 491,
  511-512. See also transition metal
  compounds chemical bonding
energy decomposition approach to bonding in
  f block compounds 338-339
- towards 32-electron rule 340-341
- U-N and U-O bonding in uranyl(VI)
    complexes 339-340
entanglement measures for single-and
  multireference correlation effects
  239 - 242
ethylene and acetylene complexes 190,
  192 - 195
exchange repulsion (EXR) 479, 481, 482
```

# f

Fe<sub>2</sub> complexes 264–265 Fermi's golden rule expression 272 Fermi level and electron counting 449–451 ferrocene and bis(benzene)chromium 199–203 frustrated Lewis pairs (FLP) 482, 483 frustrated recoupled pair bond 57 fullerenes 400–401

### g

gauge-including magnetically induced current (GIMIC) 424 generalized valence bond (GVB) 226 group-13 diyl complexes 195–199 group orbital density of states (GODOS) 299, 300

# h

halogen bonding 526, 529, 531, 532 Hammett and Hammett-Brown substituent constants 363-365 heavy main-group atoms multiple bonding 25 - 27 – comparative bonding analysis of N<sub>2</sub> and P<sub>2</sub> with N<sub>4</sub> and P<sub>4</sub> 29-32 - diatomic molecules bonding analysis 27 - 29- tetrylynes HEEH (E=C-Pb) -- bonding analysis 32-34 -- different structures 34-41 – energy decomposition analysis 41–45 hexamethylethane derivatives 493-494 high electronegativity and small size of 2p-elements 4 hybridization defects 4–7 homoaromatic molecules 403-405

homonuclear diatomic molecules 255-258 honorary d-elements 19-20 Hückel and Möbius structures 401-403 hybridization defects influence on magnetic resonance parameters 14-15 hydrogen bonding 501-502 - fundamental properties 502-504 - in biological molecules 506-507 - theoretical descriptions - - ab initio and density functional theory calculations of water dimer 510-511 - - electron density distribution analysis 513-514 - - electrostatic and orbital interactions 509 - 510 – energy decomposition analysis 511–512 - - improper, blueshifting hydrogen bonds 516 – resonance-assisted hydrogen bonding 515 - - topological analysis of electron density and electron localization function 514 -- valence bond 508-509 - with varying strengths 504-506 hydrogen bonding 524, 529, 530, 531, 533 hydrogen bridge 503 hyperconjugation 370  $-\beta$ -effect 371-372 - in ethane and ethane-like compounds 370-371 hypervalency 15, 16, 17, 21 hypoelectronic metalloboranes 136-138

#### i

inert-pair effect and dependence on partial charge of central atom 7-10 inorganic aromatic compounds 421-422 - aromaticity and antiaromaticity 422-426 - conventional aromatic and anti-aromatic inorganic molecules 426 – – aromatic  $P_4^{2-}$ ,  $P_5^-$ ,  $P_6$  and analogs 428-430 – inorganic B<sub>3</sub>N<sub>3</sub>H<sub>6</sub> borazine and 1,3,2,4-diazadiboretiidine B<sub>2</sub>N<sub>2</sub>H<sub>4</sub> 427-428 - unconventional aromatic and antiaromatic inorganic molecules 430-431  $--\sigma$ -aromatic and  $\sigma$ -antiaromatic species 431-432  $-\sigma$ - $/\pi$ -aromatic,  $\sigma$ - $/\pi$ -antiaromatic, and species with  $\sigma$ -/ $\pi$ -conflicting aromaticity 432-436

 $- - \sigma -/\pi -/\delta$ -aromatic,  $\sigma -/\pi -/\delta$ -antiaromatic, and species with  $\sigma -/\pi -/\delta$ -conflicting aromaticity 436–440 insulators 450, 456–459 intermolecular H bond 503 intermolecular perturbation theory (IMPT) 532

#### k

Kitaura–Morokuma (KM) energy decomposition analysis 511–512 Kohn–Sham density functional theory (KSDFT) 338, 340, 342, 353

#### I

lanthanides and actinides 337 - covalency and actinides 342-347 electron localization function f block applications 341-342 - energy decomposition approach to bonding in f block compounds 338 - 339-- towards 32-electron rule 340-341 - - U-N and U-O bonding in uranyl(VI) complexes 339-340 - multi-configurational descriptions of bonding in f element complexes 347 -- bonding in actinyls 349-350 – oxidation state ambiguity in f block metallocenes 350-353 – quintuply bonded actinide dimer 347-349 - technical issues 338 Larmor-Langevin equation 388, 391-393 local density of states (LDOS) 272, 277, 284, 297-299, 305, 306, 310 localized bonding schemes for bonding in polyhedral boranes 119-122 localized molecular orbitals 487 local spin 230-233 London dispersion 477. See also dispersion interaction energy theory 480–485 lone-pair bond weakening effect (LPBW) 13

# m

main-group elements chemical bonding 1-2
2p shell accounts radial nodes lack 2-4
- high electronegativity and small size of 2p-elements 4-7
- hybridization defects influence on magnetic resonance parameters 14-15 - - inert-pair effect and dependence on partial charge of central atom 7-10 – multiple-bond paradigm and bond strengths 13-14 - - stereo-chemically active versus inactive lone pairs 10-12 - honorary d-elements 19-20 outer d-orbitals in bonding 15–17 secondary periodicities 17–19 matrix product states (MPS) 227, 228 metallabenzenes 376-378 metal-metal multiple bonding 211-213 - with multireference quantum chemical bonds modeling 253 - - Cr<sub>2</sub>, Mo<sub>2</sub>, and W<sub>2</sub> containing complexes 259 - 263- - effective bond orders 253-254 -- Fe2 complexes 264-265 – homonuclear diatomic molecules 255-258 - - multiple bond in Re<sub>2</sub>Cl<sub>8</sub><sup>2-</sup> 254-255 metal particle composition and size dependence - alloving 303-305 - particle size dependence 305-310 Mg~5B44 electronic structure 143-144 mno rule 126-134 molecular electrostatic potential (MEP) 523-528.533 molecular Wankel motor 436 monovalent metal clusters highest spin states bound triplet pairs 149-150 – calculation methods and details 170 - NPFM bonding -- in coinage metal clusters 161-167 – generalization in <sup>n+1</sup>Li<sub>n</sub> clusters 156-161  $- - {}^{n+1}Li_n$  clusters 152–154  $- - {}^{n+1}\text{Li}_n(n = 2-10)$  series 152 -- orbital cartoons 154-156 – resonating bound triplet pairs 167-168 - prototypical bound triplet pair in <sup>3</sup>Li<sub>2</sub> 150, 151 - VB configuration count ad expressions for de for NPFM clusters 171-172 - VB wave function symmetry assignment 170 - 171Mott-Hubbard localized states 456-457 Mott transition 458 multicenter indices (MCI) 424

multi-configurational descriptions of bonding in f element complexes 347

- bonding in actinyls 349-350

- oxidation state ambiguity in f block metallocenes 350-353
- quintuply bonded actinide dimer 347–349 multiple-bond paradigm and bond strengths 13 - 14

### n

natural bond orbital (NBO) 425, 525, 530 natural energy decomposition analysis (NEDA) 512 natural-orbital occupation numbers 223 natural orbitals 348-352, 353 Newns-Anderson model 272, 282, 283 NMR chemical shifts 391-392 noncovalent interactions (NCIs) 477, 485, 486, 489-491, 533 no-pair ferromagnetic (NPFM) bonding 171 - 172- in coinage metal clusters 161 -- structures and bonding 161-163 -- valence bond modeling 163-167 – generalization in <sup>n+1</sup>Li<sub>n</sub> clusters 156 - - <sup>n+1</sup>Li<sub>n</sub> patterns VB modeling 158–161 - - VB mixing diagram representation of bonding in <sup>3</sup>Li<sub>2</sub> 156, 157 - <sup>n+1</sup>Li<sub>n</sub> clusters 152-154  $-^{n+1}Li_n(n = 2-10)$  series 152 - orbital cartoons 154-156 resonating bound triplet pairs 167–168 nucleus-independent chemical shift (NICS) 396, 423-424

#### 0

occupation numbers (ONs) 425 open-shell transition-metal complexes 219-220

- qualitative interpretation
- -- atoms in molecules 237-238
- -- bond orders analysis 235-237
- -- broken spin symmetry 233-235
- - entanglement measures for single-and multireference correlation effects 239-242
- --local spin 230-233
- spin density distributions 243
- -- multiconfigurational study 245-246
- -- one-determinant picture 243-245
- theoretical foundations 220-221
- ab initio multireference approaches 224-229

 – ab initio single-reference approaches 223-224 – configuration interaction ansatz 222-223 - - density functional theory for open-shell molecules 229-230 -- electronic structures definition 221-222 orbital interactions 75-78, 81, 82, 85, 86, 87, 88, 96, 98, 101, 103 104, 106, 179, 180, 183, 186, 189, 193, 195, 198-200, 208, 210, 212, 213 organometallic compounds 404, 405-406 outer d-orbitals in bonding 15-17 overlap population density of states (OPDOS) 274, 275, 291, 293, 296-298

#### р

partial density of states (PDOS) 278, 280-281-283, 294, 295, 297, 300 particle size dependence 305-310 Pauli repulsion 330-331 Peierls distortions 451-452 pericyclic reactions 406, 409, 411, 413 phosphane complexes and n-heterocyclic carbine complexes 187-190 point-charge models 531 polar flattening 525 polar metallic solids 459-462 purely electrostatic models 530-531 pyridine, phosphabenzene, and silabenzene 398-399

#### q

quantum theoretical treatment 392-397 quantum theory of atoms-in-molecules (QTAIM) 345-347, 514-516

 $\operatorname{Re}_2\operatorname{Cl}_8^{2-}$  multiple bond 254–255 recoupled pair bond dyad 59 recoupled pair bonding in hypervalent molecules 49-50 - comparison with other models 64 - - democracy principle 67 -- diabatic states model 66-67 -- Rundle-Pimentel 3c-4e model 64-65 - multireference wavefunction treatment of bonding 50-53 - SF and OF low-lying states 53-57 –  $SF_2$  and  $OF_2$  (and beyond) low-lying states 58 -- OF<sub>2</sub> triplet states 62-63  $--OF_2(X^1A_1)$  62  $--SF_2(a^3B_1)$  59, 61

 $\begin{array}{l} -- \mathrm{SF}_2(\mathrm{b}^3\mathrm{A}_2) & 61-62 \\ -- \mathrm{SF}_2(\mathrm{X}^1\mathrm{A}_1) & 58-59 \\ -- \mathrm{SF}_3 & \mathrm{and} & \mathrm{SF}_4 & 63-64 \\ -- \mathrm{SF}_5 & \mathrm{and} & \mathrm{SF}_6 & 64 \\ \mathrm{relativistic} & \mathrm{effects} & 2, 8, 11, 17-19 \\ \mathrm{resonance-assisted} & \mathrm{hydrogen} & \mathrm{bonding} & 515 \\ \mathrm{ring} & \mathrm{current}. & See \ \mathrm{aromatic} & \mathrm{compounds} & \mathrm{and} \\ \mathrm{transition} & \mathrm{states} & \mathrm{magnetic} & \mathrm{properties} \\ \mathrm{Rundle-Pimentel} & 3c-4e \ \mathrm{model} & 64-65 \\ \end{array}$ 

s

scandide contraction 18, 21 secondary periodicities 17-19 semiconductor 450, 451, 459 semimetals 451 SF and OF low-lying states 53-57 SF2 and OF2 (and beyond) low-lying states 58 - OF<sub>2</sub> triplet states 62-63  $-SF_2(b^3A_2)$  61–62  $--OF_2(X^1A_1)$  62  $-SF_2(X^1A_1)$  58–59  $--SF_2(a^3B_1)$  59, 61 - SF<sub>3</sub> and SF<sub>4</sub> 63-64 - SF<sub>5</sub> and SF<sub>6</sub> 64 single-orbital entropy 239 solids 445-447 - bonding 458  $- - Ba_7Ga_4Sb_0 = 470 - 473$ - - covalent bonds in polar metallic solids 459-462 – crystal versus electronic structure 466 - 470 – electronic localization 462–466 - electronic structures 447 - - Bloch orbitals, crystal orbitals, and band structure 447-449 -- density of states and analysis 453-456 -- electronic localization 456-458 - - Fermi level and electron counting 449-451 -- Peierls distortions 451-452 spin density distributions 243 - multiconfigurational study 245-246 - one-determinant picture 243-245 stereo-chemically active versus inactive lone pairs 10-12 steric crowding and labile molecule 493-494 styx formalism 120, 122 substituted ethenes 492-493 supermolecular density functional theory 488-490

supermolecular wave function theory (WFT) 486–488 surface molecule limit 274 surface reactivity 269 symmetry-adapted perturbation theory (SAPT) 490, 491, 530, 531

### t

tensor network states (TNSs) 228 tetrylynes HEEH (E=C-Pb) - bonding analysis 32-34 - different structures 34-41 – energy decomposition analysis 41–45 thermochemistry. See dispersion interaction three center, four electron model. See Rundle-Pimentel 3c-4e model through resonance 364 time-dependent density functional theory (TDDFT) 484, 485 time reversal symmetry 449 TIP3P model 509 topological rules 119 transition metal compounds chemical bonding. See also open-shell transition-metal complexes 175-176 - carbonyl complexes 181-187 - cluster, complex, and electron-sharing compound 203-211 - ethylene and acetylene complexes 190, 192 - 195- ferrocene and bis(benzene)chromium 199 - 203- group-13 diyl complexes 195-199 - metal-metal multiple bonding 211-213 - phosphane complexes and N-heterocyclic carbene complexes 187-190 - valence orbitals and hybridization in electron-sharing bonds 177-181 transition metal surface bonding and reactivity quantum chemistry 269-271 - adatom adsorption energy dependence on coordinative unsaturation of surface atoms 276-283 – adatom adsorption energy as function of metal position in periodic system 284-286 - - adsorbate coordination in relation to adsorbate valence 301-303 – molecular adsorption and CO adsorption 286-296 -- surface group orbitals 296-301 - adsorbate bond activation and formation - - different metal surfaces reactivity 317, 318-321

transition metal surface bonding and reactivity quantum chemistry ( <i>contd</i> .)	van der Waals (vdW)    477, 478, 481 – density function (vdW-DF)    488–490
quantum-chemical view of bond activation 321-328	van Hove singularity 453 VSEPR model 10, 19, 179
<ul> <li>analysis 328–333</li> <li>elementary quantum-chemical model 272–276</li> <li>lateral interactions and reconstructions 310–317</li> </ul>	<b>W</b> Wade's rules 114–119, 122 Woodward–Hoffman rules 330
<ul> <li>metal particle composition and size</li> <li>dependence</li> <li>alloying 303–305</li> </ul>	<b>y</b> ylides 72
<ul> <li>– particle size dependence 305–310</li> </ul>	<b>z</b> Zintl phases 456, 458, 459, 468, 470–474

valence bond 508–509 valence orbitals and hybridization in electron-sharing bonds 177–181