Ab initio level calculations, 67, 69, 70

Acecorannulylene, 239

acid-catalyzed aldol trimerization, of acecorannulenone, 247–251
alo d cyclotrimerization, 248
bowl-to-bowl inversion, 248
conformational isomers of C₆₆H₂₄ trimer, 247
¹H NMR shifts for C₆₆H₂₄ trimer, 249, 250
variable-temperature ¹H NMR of C₆₆H₂₄ trimer, 250
conversion to acecorannulenone, 244–247
epoxide isomerization route to, 245
mild epoxide to ketone isomerization, 245
one-step Wacker oxidation route to, 247
oxymercuration-demercuration of acecorannulylene, 246
two-step route to, 246
“stitch up” acecorannulenone trimer, 251–255
FVP syntheses of circumtrindene, 251
mass spectrum of products, 252
oxidative cyclodehydrogenation, of hexaphenylbenzene, 252
reductive couplings of helicene moieties, in partially stitched-up, 255
indenocorannulene, 254
reductive cyclodehydrogenation, of helicene, 253
synthesis, 239
Cheng and Scott’s pyrolytic synthesis, 240
FVP syntheses, 241
hexakis(dibromomethyl) fluoranthene, 242
key factors, 243
Rabideau’s and Siegel’s nonpyrolytic syntheses, 240
Rabideau’s pyrolytic synthesis, 240
unsuccessful cyclization route to, 242
Aacenaphthylene reaction, 218
Acetate thermolysis, see Thermolysis
Aldol cyclotrimerization of acecorannulenone, 248
of structurally related acenaphtylene, 247
using combination of p-TsOH H₂O and benzoic acid, 247
Alkyne cycloaddition, 222
All-Z-benzannulenes, 312
complexes, 320
conformational analysis, 325–328
molecular structures, 320
photocyclization reaction, 328–330
retrosynthetic analysis, 315
structures and dynamic behaviors, 318–325
synthesis, 314
X-ray crystallographic analysis, 320
All-Z-cyclophanetriene, 330
  oxidative cyclization, 332, 334
  properties, 332
  structure, 332
  synthesis, 330–332
Aluminum chloride, 243
Aluminum cyclohexide, 16
Annelated corannulene, see Corannulene
Annulene-within-an-annulene model, 69
Anthracene, 16, 63, 207, 210, 264, 266,
  355, 393
  9-Anthracenyl complex, bromination
  chemistry, 224
Anthranilic acid, 12
Arene-perfluoroarene interactions, 176
  (2,2)-Armchair nanotube, 264
  4,4-Armchair nanotube section, 285
Aromatic belts
  CNT growing strategies, 279–286
  brickling, 281–283
  stacking and host-guest stacking,
  283–286
  from concave precursors synthesis,
  261–263
  nanotube endcaps synthesis, 260–261.
  See also Carbon nanotube (CNT)
  as nanotubes sections, 259
  by REM synthesis, 264–279
Aromatic belts, strategy for synthesis,
  390–396. See also VID reaction
  conversion of aromatic board into, 395
  $D_{6h}$-symmetric Vogtle belt, 390
  failed approach to Vogtle belt, 391
  selection of targets, 396
  tetrafunctionalized aromatic boards
  synthesis, 392, 394
Aromatic stabilization energy (ASE),
  371
Aromatization, 262, 299, 343, 345, 346,
  352, 392
A (2,11)teropyrenophane, 387–390
  crystal structure, 389
  synthesis of
  $[n]cyclophanes, 387
  1,1,8,8-tetramethyl[8](2,11)
  teropyrenophane, 388
  Barbier reactions, 51
  Basis set superposition error (BSSE), 20, 141
Beltlike compounds, 274
Belt-shaped $\pi$-conjugated molecules,
  311
Benzannulated enediyne, 42
Benzannulated enyne-allenes, 41
  synthesis
  10-(1,1-dimethylethyl)-5-phenyl-11$H$-
  benzo[b]fluorene via, 42
  methods for, 41
Benzannulenes, 314
  DBCOT, analog for, 318
  synthesis, 314–316, 319
Benzene, 2, 4, 6, 30, 71, 180, 270, 326, 332,
  335, 374, 381, 393, 395
Benzene-H$_2$-pentaindenocorannulene
  complex, 144
Benzofluorene, 42, 43, 46
Benzofluorenyl diketone, 56
Benzylic chloride, 243
Benzylbromides, 11
Benzylic chloride, 243
Benzyn–Stevens rearrangement, 392
Bertozzi’s approach, 263
Bicorannulene dianion, 75–76
  highest occupied molecular orbital, 76
  reduction with potassium metal, 75
  octaannion, 76–77
  reduction with lithium metal, 77
  reversibility of binding, 77
Binding energy, 22
  2,2'-Biphenyldiyl nickelacycles, 220
Bipolar longitudinal eddy-current delay
  (BP-LED), 67
Bis(benzocorannulene) cyclooctadiene,
  31–32
  alternative synthetic routes to, 31
  crystal structure, 33–34
  intramolecular $\pi$–$\pi$ stacking
  interaction, 33
  twist-boat conformer, 33
Bicorannulenebarrelene, 17
  alternative tethers to incorporate, 18
  endo-endo conformer, 18
  endo-endo variant, 18
  MM2 geometries, 18
Bis(benzocorannulene)barrelene, 24
Bis(fluoranthene barrelene), 17
2,6-Bis-2-pyridyl-1,2,4,5-tetrazine, 14
Bistriazolinedi anthracene, 264
Bodwell’s approach, 263
Bowl-shaped π-conjugated molecules, 96, 97
Bowl-shaped pincers, 2
Bowl-shaped polyaromatic hydrocarbons, 187
coordination preferences
dinuclear metal complexes, 163–174
metal complex nuclearity, 157–180
mononuclear metal complexes, 157–163
polynuclear metal complexes, 178–180
trinuclear metal complexes, 174–178
Bowl-to-bowl inversion barriers, 97
9-Bromoanthracene, 264
2-Bromobenzaldehyde, 317, 318
Bromocorannulene, 12, 13, 108
complex, 168
Bromodiester, 393
2-Bromo-4,5-diethoxybenzaldehydes, 334
4-Bromo-1-indanone, 54, 58
o-Bromophenol, 13
o-Bromotrimethylsilyl ether, 14
Buckminsterfullerene, 3
Buckybelts, 347
Buckybowl-like nanographene, 95
Buckybowls, 63
anions, 63
characterization, 65–68
preparation, 64–65
stabilization, 64–65
donoexo-coordination, schematic
representation of, 158
complexes, 179
electrochemical studies, of reduction, 68
family of buckybowls, 64
applications, 64
Jahn–Teller distortion, 65
LUMO energy levels, 65
synthesis, 7–12
Buckycatcher C_{60}H_{28}
major uses of, 36–37
synthesis, 19
two-photon absorption (TPA) process, 37
Buckycatcher complexes, with C_{60}
and C_{70}, 22
association constants, 24
binding energy, 25, 27
carbon–carbon distances, 23, 24
C_{70} complexation by, 27–29
changes in chemical shifts, 24, 25
C_{2v} symmetry of corannulene pincers, 23
entropy and solvation penalties,
influencing assemblies with
fullerenes, 25
NMR titration experiment, 24, 26
π–π stacking of bowl-shaped conjugated
carbon networks, 26
TBCOT scaffold align corannulene
pincers, 24
Buckycatcher-fullerene complexes
in photovoltaic devices, 36
Buckyribbon, chemical structure, 349
Carbomethoxymethyl protons, 17
Carbon-heteroatom bond, 217
Carbon nanotube (CNT), 63, 95, 291
“brickin” strategies, 279
categories, 235
achiral, 235, 236
armchair, 235, 236
chiral, 235, 236
multiwalled, 235
zigzag, 235, 236
conventional synthesis, 274
cycloparaphenylenne as possible
unit, 292
electronic properties, 237
growing strategies, 279–286
knitting, 260
mechanical properties, 292
as new challenges for organic
synthesis, 292
properties depending on structure, 293
stacking strategies, 280
structure, 259
template synthesis approaches,
260–279
wet chemical synthesis, 259
Carbon nanotubes, 264
C_{60}-based molecular systems, 95
C_{84}-fullerene hemisphere, 261
formation, 262
C_{60}-fullerene subunits, 159
Chemical vapor deposition (CVD),
281
C_{30}H_{12} geodesic polyarene, 88
reduction with potassium metal, 88
Collision-induced dissociation (CID) mass spectrometry, 137
Colloidal metal-catalyzed decomposition, 222
Colloid catalyst, 221
Colloid-catalyzed reactions model, 223
$\eta^1$ Complexes
  by metathesis, 212
  by oxidative addition, 210
Co 1-naphthyl complex, 214
Concave-convex π-π interactions, 311
Concave-selective complexation, 197–198
π-Conjugated molecular tweezers, 313
π-Conjugated molecules planar, 1
Coordination modes
  identified by X-ray diffraction, 162
  of π bowls in structurally characterized mononuclear metal complexes, 162
  structurally characterized [Rh$_2$(O$_2$CCF$_3$)$_4$] complexes, π bowls in, 172–173
Copper-catalyzed etheration, 13
Corannulene-based synthons synthesis, 12–15
1,5-Corannulene cyclophane, 145
Corannulenes, 2, 3, 135, 163–167, 175
annelation, 78
Ball-and-Socket Li$^+$-mediated stacking, 77–78
Barth–Lawton synthesis, 7–8, 49
calculated and experimental electron affinities, 138
ionization potentials, comparison, 137
carbenoid coupling, of octabromide, 11
complexes, formed by C–X oxidative addition, 211
coordination preferences, 167
decasubstituted derivatives, synthesis, 151
dianion, 70–71
dimerization, 74
dipole moment, 140
exo-bound transition metal $\eta^6$ complexes, 161
Friedel–Crafts acylation, 239
halogenation, 150
hydrogen adsorption vs. experimental measurements, 144
hydrogen uptake by, 143, 145
indenoannulation, 177
LUMO energy levels, 68, 106, 152
π-metal complex, 159
monoanion, 69–70
monobromination, 147
monosubstituted derivatives, synthesis, 147
multiethynylcorannulene derivatives, 152
nickel-powder-induced formation of corannulene core, 11
open-shell systems based on, 105–106
diradical system, 114–120
monoradical systems, 106–114
phenalenyl-fused corannulene, 120–124
penta-1,5-butyl-corannulene, 74
pentasubstituted derivatives, synthesis, 151
POAV angles, 116
reactions, 174
reduction pathway, 69
potentials, 138, 139
spectroscopic characterization, 68–69
ring system, 145
sandwiched molecule, 175
Scott’s FVP synthesis, 9
Siegel’s “wet” synthesis, of 2,5-dimethylcorannulene, 9
steady-state fluorescence measurements, 144
structure, 136, 142
tetraanion, 72–74
isomers of supramolecular heterodimer, 78
trianion, 71–72
valence bond structure, 69
Corannulene tetraaldehyde, 10
1,5-Corannulenylcyclophane, 142
Corannulene by anthranilic acid route, 13
from bromocorannulene, 13
mild generation from 2-TMS-corannulennyl triflate, 14
Corey–Winter reaction, 315, 317
of cyclic pinacol, 314
[CpFe(sumanene)]PF₆ synthesis, 198
Cu(II) chloride-promoted coupling, 54
Curved pincers, 1
Curved π-radical, 98
C₃ᵥ [6,6]SWNT endcap, retrosynthetic analysis, 238, 239
Cyclic voltammetry (CV), 68
measurements of anion R₆C₆₀⁻, 103
Cyclooctadiene (COD) tether, 30
Cyclooctatetraene (COT), 312, 313
tethers, 30
Cyclopaphenylene ethynlenes, 312
Cyclopaphenylene, 291
benzenoid vs. quinoid character, 297
[8]cyclopaphenylene optical characterization, 307
Stokes shift, 306
synthesis by reductive elimination strategy, 305–306
[12]cyclopaphenylene, 303
final steps, 305
Itami’s synthesis, 304
selective synthesis, 303–305
strain energies for cyclization, 304
Herges’ synthesis of picotube, 296
macrocyclic precursors Jasti’s synthesis, 298
prone to migration under acidic conditions, 299
π system, 294
timeline for synthesis, 294
early studies related to, 294–297
first synthesis and characterization, 298–303
as unit of armchair CNT, 292
Vögte’s proposed strategies for synthesis, 295
Cyclopenta[bc]corannulene, 80
reduction with lithium metal, 81
tetraanion dimer, 80
lithium cations to interact with, 81
peri-annelation with 5MRs, 81
Cyclopentacorannulene, steady-state fluorescence measurements, 144
Cyclopentacorannulene, 8
absorption spectrum, 146
Cyclopentadienone, 16, 49
Cyclopentadienyl anion-type electronic structure, 103
Cyclopentadienyl radical, 103
Cyclopentaindenophenylene bowl-shaped, synthesis of, 45
Cyclophanediene, 374, 379, 383, 384, 387, 388
Cyclophanes, 63, 263, 312, 368, 369, 390
Cyclophenacene, 312, 328, 330, 333, 334, 339, 360

Decakis(phenylthio)corannulene, structure, 153
cyclic voltammetry, 153
Decarboxylation reaction, 49
of fluorenone, 216
of naphthoyl complexes, 213
Density functional theory, 5, 67, 165, 167, 170, 178, 189, 301
Deoxygenation, 14, 20
ortho-Deprotonation, 12
Dess–Martin oxidation, 317
Dialdehyde, 334, 360, 388
insoluble linear, 331
Lindlar catalyst afforded, 318
macrocyclization, 316
preparation, 317, 318
Diarylacetylene, 315
hydration, 315
Dibenzo[a,g]corannulene, 79, 80
Dibenzo[a,g]cyclopenta[k]corannulene, 80
Dibenzocyclooctadiene tethers, potential clips with, 30–33
Dibenzocyclooctadiyne, 18, 19
Dibenzocyclooctatetraene (DBCOT), 313, 318, 334
ring inversion, 319
Dibenzocyclooctatetraene tethers, potential clips with, 30–33
Dibromoethylen derivative, 317
ortho-Dichlorobenzene, 247, 248
Dicorannulenobarrelene clip, 22
Dicorannulenobarrelene dicarboxylate, 16
1,8-Dicorannulenyloctane, 74, 78
reduction with lithium metal, 75
1,8-Dicorannulenyloctane tetraanion, 70
1,2-Didehydrocorannulene, 12, 14, 30
Diels–Alder (DA) chemistry, 344
Diels–Alder cycloaddition reaction, 12, 14
appropriate diene generating tetra benzocyclooctatetraene scaffold, 19
to 1,2-benzoquinone, 16
with 2,5-dihydrofuran, 49
of isocorannulenofuran, 15
with benzocyclobutadiene, 30
Diels–Alder products, 269
Diels–Alder reactions, 262, 265, 282, 283
Diffusion-ordered spectroscopy (DOSY), 67
Dihydrocyclopenta corannulene, 46
2,5-Dihydrofuran, 49
Diindenol[1,2,3-bc:1,2,3-hi]corannulene, 79, 80
Dimerization, 72, 73, 78–81, 80, 104
leads to cyclobutadienes, 361
of monoaldehyde, 318
for neutral radical species, 105
of cis-stilbene derivative, 317
Dimetal complexes, 164
Dimethylacetylenedicarboxylate, 17
Dimethylation, 49
2,4-Dimethylcarbonohydrazide, 108
2,5-Dimethylcorannulene, 9
10-(1,1-Dimethylthethyl)-5-phenyl-11H-benzo[b]fluorene, 42
1,3-Dimethyl-2-phenyl-1,3,2-diazaphospholidine (DMPD), 316
1,7-Dioxa[7](2,7)pyrenophane, 378
Dipole-dipole attraction, 7
Dipole moment, 139
Diradical system, 114–120
canonical resonance structures, 115
chemical structure, 115
electronic spin structure, 117
glass-phase ESR measurements, 117
intramolecular magnetic interaction, 117
molecular structure, 116
NOON analysis, 120
spin density distributions, 118, 119
Direct X-ray diffraction studies, 163
Dirhodium units η5-rim coordination of, 164
Dithiacyclophanes, 369
Diynetetraester, 393
DNA-nanotube interactions, 237
Dynamic molecular tweezers (DMTs), 334.

See also Molecular tweezers composed of two DBCOT units, 334
stepwise reactions, 334, 335, 337–339
syn form on complexation, 334
\(^1\)H NMR titration, 336
thermochromic behavior, DDQ complexes, 338

Echinomycin, 1
Electron affinity, 137–139, 302
Electron correlation, 137
Electronic device fabrication, 206
Electron spin resonance (ESR) spectroscopy, 67
Electrostatic ion-dipole interactions, 178
Electrostatic potential surfaces (EPSs), 335
Endoxides, 14
Epoxides, 244, 245
1-Ethynyl-2-(2-phenylethynyl)benzene, 42
Euler’s theorem, 3
Exchange NMR spectroscopy (EXSY) for buckybowl anions, 66, 88
for determining energy barrier for, 67, 87
estimation of isomerization rate, 193, 199

Fast-atom bombardment (FAB) mass spectrometry, for sumanene, 198
Ferromagnetism, 95
Field effect transistor (FET) methods, 200
Flash vacuum pyrolysis (FVP), 188, 239, 261, 275, 283
Fluoranthene, 8
Fluoranthene-7,10-diacetic acid, 8
9-Fluorenone, 42
Fluoride anions, 13
Fourier transform (FT) ESR, 68
Friedel–Crafts acylation, 49, 122, 239, 243
Friedel–Crafts alkylation, 273, 276, 387
Friedel–Crafts cyclization, 8
Frontier molecular orbitals (FMOs), 165, 168
Fullerenes, 3
applications, 36–37
buckybowl-fullerene complexes, 4
computational considerations
  dipole moment, 139
electron affinity, 137–139
  ionization potential, 136–137
  spectroscopy, 139–140
concave-convex stacked supramolecular assemblies of, 16
corannulene relationship with, 3
experimental and calculated properties, 135–136
fragments, 3
fullerene cages, 15, 18, 23–27, 29
fullerene receptor design, 5
hydrogen complex, 140–142
LUMO energy level, 98, 138, 152
molecular clips and tweezers interaction with, 36
molecular structure and p orbitals, 96
open-shell systems based on, 98
  neutral radicals, 103–105
  radical anion species, 98–103
photophysical properties
corannulene and cyclopentacorannulene, 142–146
highly substituted corannulene, 149–152
monosubstituted corannulene derivatives, 146–149
reductions and oxidations
corannulene and corannulene derivatives, electrochemistry, 152–153
corannulenes with alkali metals, reduction, 153–154
separation in crystal, 23
structure, 136
tweezer-fullerene complexes, 3
Fully unsaturated, beltlike compounds, 344
Fully unsaturated, double-stranded hydrocarbon cycles, 343
Diels–Alder approach, 344–358.
  See also Thermolysis
diatomic chemical transformations, with dihydrate, 352
conversion of dihydrate into, 351
double-stranded structures, 345
for first formal cyclacene precursor, 346
for high-molar-mass ladder polymer, 345
macrocycle, 345
tetrahydrate, synthetic sequences, 350
synthetic tools in field of double-stranded belts, 358
compounds in regard to cyclo[n]phenacene synthesis, 359
Fully unsaturated, double-stranded hydrocarbon cycles (Continued)
double-stranded cycles of cyclo[n]phenacene type, 359
key sequence, 362
McMurry reaction, 358
possible routes into cyclic oligo(ortho-
arylenevinylene), 360
1-Functionalized naphthalenes,
cyclometallation products for, 209

Gauge-independent atomic orbital (GIAO) method, 67

Graphene
molecular structure and p orbitals, 96, 97
sheet, 206, 275, 293
Grubbs and Schrock catalysts, 265

Harmonic oscillator model of
aromaticity, 372
Hemifullerene, 171–174
charge distribution, 89
analysis, 88
concave-concave tetrameric aggregate, 88
DFT calculations, 88
ligands, 174
pyramidalization, 88
reduction with potassium, 88
supramolecular aggregation, 89

Herges’ approach, synthesis of aromatic
belts, 265

Heterosumanenes
heteroatom functionalities, 196
synthesis, 197

Heteroatom functionalized naphthalenes,
cyclometallation, 207
Hexabenzocoronene, 211, 251, 252, 261, 262
Hexahydrosumanene, 189

Hexakis(dibromomethyl)-fluoranthene, 239,
241, 242
1,3,4,6,7,10-Hexamethylfluoranthene, 243
Hexaphenyldibenzene, 252
High-dilution apparatus, 244
High-molar-mass ladder polymer
DA route to, 345
High-performance liquid chromatography
(HPLC) analysis
chiral stationary phase, 273
tetraphenylenes, 221

High-temperature flash vacuum pyrolysis, 275
High-temperature methods, of nanotube endcaps, 260, 264
Hofmann elimination, 374, 383, 394
HOMO-LUMO overlap, 190, 200
Host-guest supramolecular chemistry, 3
Hydride complex, 208, 219
Hydrocarbon, see Polycyclic aromatic hydrocarbons

Hemifullerene, 171–174
charge distribution, 89
analysis, 88
concave-concave tetrameric aggregate, 88
DFT calculations, 88
ligands, 174
pyramidalization, 88
reduction with potassium, 88
supramolecular aggregation, 89

Herges’ approach, synthesis of aromatic
belts, 265

Heterosumanenes
heteroatom functionalities, 196
synthesis, 197

Heteroatom functionalized naphthalenes,
cyclometallation, 207
Hexabenzocoronene, 211, 251, 252, 261, 262
Hexahydrosumanene, 189

Hexakis(dibromomethyl)-fluoranthene, 239,
241, 242
1,3,4,6,7,10-Hexamethylfluoranthene, 243
Hexaphenyldibenzene, 252
High-dilution apparatus, 244
High-molar-mass ladder polymer
DA route to, 345
High-performance liquid chromatography
(HPLC) analysis
chiral stationary phase, 273
tetraphenylenes, 221

High-temperature flash vacuum pyrolysis, 275
High-temperature methods, of nanotube endcaps, 260, 264
Hofmann elimination, 374, 383, 394
HOMO-LUMO overlap, 190, 200
Host-guest supramolecular chemistry, 3
Hydride complex, 208, 219
Hydrocarbon, see Polycyclic aromatic hydrocarbons

Indenoannulation, 169, 170, 177
Indenocorannulenes, 78, 253. See also
Corannulene
anions of, 78–79
reduction process, of diindenoc[1,2,3-
bc:1,2,3-hi]corannulene, 79
stepwise reduction with potassium metal, 79
Infrared spectrum, of corannulene, 139, 140
π–π Interactions, 3, 335
stacking in curved surface systems, 4–5
between bowl-shaped PAHs, 4
between corannulene and C60, 5
buckybowl-fullerene complexes, 4
rim substituent-fullerene interactions, 4
STM study, for corannulene-C60 complexes, 5
X-ray crystallographic data, 5
theoretical models, 5–7
conformations of π–π stacked corannulene dimers, 6
density functional theory (DFT), 5–7
Hartree–Fock molecular orbital (MO) methods, 5
Interlayer distance (ILD), between
corannulene units, 142, 145
Intermediate neglect of differential overlap/configuration interaction
(INDO/CI) calculations, 146
Intramolecular Mizoroki–Heck reactions, 194
Iodonorbornene derivative, regioselective
cycotrimerization, 195
Ionization potential, 136–137, 301
of corannulene and curved polyarenes, 253
for paraphenylenes, 302
Isobenzofurans, 14
Isocorannulenofuran, 12, 14, 30
Isofuran, 31, 32
Isolated pentagon rule (IPR), 238
Isomerization
  of kinetic product, 210
  mild epoxide to ketone, 245
  ruthenium-catalyzed, 241
  trideuteriosumanene, 192, 193
valence, 370, 371, 374

Kammermeierphane, 270
Koopman’s theorem approach, 137

Laser desorption ionization time-of-flight mass spectroscopy (LD-TOF-MS), 312
Lewis acidic complexes, 163
Lewis acids, 165, 353
Lewis base, 168
Lindlar’s catalyst, 315, 318
Lithium acetylide-ethylenediamine complex, 56
Lithium acetylides, 42, 56
Lithium diisopropylamide (LDA), 54
Lithium naphthalenide, 300
Low-temperature IR spectroscopy, 273

Macrocycle, 345
Macrocyclization, 303
MALDI mass spectrometry, 279
trans-M(1,2-corannuleny1)(PET3)2Br structure, 212
[2.2] metacyclophane, 368
syn conformation, 370
Metal-free wet-chemical process, 282–283
Metallacycle complex, 214–217
Metallation products, 210
Metal-PAC reactions
  metallacycle reductive elimination and cycloadditions, 219–223
  metal migrations, 218–219
  reactions at PAC, 223–225
Metathesis method, advantages, 213
Methoxycorannulene, 13
Methoxymethyl (MOM) derivative, 334
Methylenation, 57
Microscale gas-phase coordination technique, 163
Molecular clips, 1
Molecular dynamics calculations, 141
simulations, 142
Molecular receptors, 1, 15, 23
C60 and C70 fullerenes, 30
for fullerene cages, 26
Molecular tweezers, 1
characteristics, 1
complexity of synthesis of, 5
conformations, 2
dynamic, 334, 335
properties of π-conjugated, 313
role in identifying target molecules, 3
Molecule potential, 136–137
Moller–Plesset level, 141
Monodisperse nanotubes synthesis, amplification approach, 282
Monoradical monoanion species, 99
C60 molecule, sandwiched between nickelocene cations, 99
ESR spectrum, 99, 101
open-shell monomer, 99
X-ray crystal analysis, 99
zigzag chain arrangement, 99
Monoradical trianion species, 101
Multiwalled nanotubes (MWCNTs), 278
Nanotechnology, 135
Naphthalene C–H bond activation scheme, 207
Naphthalene systems, 209
Naphtho[2,3-a]corannulene, 79, 80
Naphthosumanenes nonpyrolytic synthetic strategy, 194
strategy for, 194
Naphthoyl complexes, decarbonylation, 213
Natural bond orbitals (NBO) theory, 67
complexes of C60 with, 35
construction, 3
equipped with corannulene pincers, 34
fullerene-hosting abilities of, 36
with more flexible 1,5-COD subunits, 31
with polar anchors, 36
research on, 33
target guests (fullerenes) with host, synthesizing, 34
tethers to incorporate into biscorannulenes, 18

INDEX 409
Neutral radical adducts, 103–105
ESR spectroscopy, 103
Neutral radical-substituted derivatives, 105
corannulene derivatives, 107–114
hyperfine ESR spectra, 109, 110
molecular structure, 110–112
synthesis, 108
Neutral radicals with benzyl moieties, 103
NiBr(PEt3)2(1,2-acenaphthylyne) preparation, 215
Nickelacycles reactions, 220
Nitroxide radicals, 105
NMR investigations, for corannulene’s surface, 160
1D NOE experiment, for bowl-to-bowl inversion, 198
Nonplanar carbon surfaces, 159
Nonplanar \(\pi\)-conjugated carbon systems, 187
Norbornadiene and acetic anhydride, 243
trimerization, by modified procedure, 190
Nucleus-independent chemical shift, 372
Octabromide, 10
Octamethylindenofluoranthene, 9
Octaphenyl-1:2,13:14-dibenzo[2]paracyclo-
[2](2,7)pyrenophane-1,13-diene, 383
Octaphenylpyrenophane, 383
Optical gap energies, 302
\(\pi\)-Orbital axis vector (POAV) analysis, 45, 190
for degree of pyramidalization for trigonal C atoms, 165
revealing six hub carbons pyramidalized to, 190
Organic field effect transistor (OFET), 200
Organic light-emitting diode (OLED) technology, 154, 208
Oxalyl chloride, 243
Oxidative cyclization of all-\(Z\)-cyclophanetriene, 332, 334
resistance of hydrocarbon, 253
PAC-yl ligands, steric footprint, 213
PAHs, see Polycyclic aromatic hydrocarbons (PAHs)
Palladium-catalyzed intramolecular arylation reactions, 59
[2]Paracyclo[2](2,7)pyrenophane, 380
1,3,5,7,9-Penta-\(t\)-butyl-corannulene, 74
Pentamethylfullerene (Me\(\_\)C\(\_\)H), 77, 78
Pentaphenylfullerene (Ph\(\_\)C\(\_\)H), 77
Perfluoro-\(\text{o}\)-\(r\)-\(t\)-\(h\)-\(o\)-\(r\)-phenylenemercury, 174, 175
Peri-metallation, 208
Phenalenyl-fused corannulene, 120–124. See also Corannulenes
bond lengths, 121
bowl inversion barriers (\(\Delta E\)) of redox species, 124
electrostatic potential surfaces, 122
\(^1\)H and \(^{13}\)C chemical shifts, 123
HOMO structures, 123
resonance structures, 123
synthesis, 122
Photoelectron spectroscopy (PES), of corannulenes, 137
Photoirradiation, 105, 329
Picotube, 272, 312

cyclodehydrogenation, 274–278
Friedel–Crafts alkylation, 276
packing and reaction, 284
properties, 273
pyrolysis, 277
reactions, 273
reactivity, 273
REM, 278–279
time-averaged \(D_{\text{sh}}\) symmetry, 273
Pinacol coupling reaction, 314, 318
Pincer complexes, 224
anthracene-centered reactions, 225
formation, 210
Planar pyrene, ASE value, 372
Platinacyle colloidal Pt catalyzed reactions, 223
preparation, 216
POAV, see \(\pi\)-Orbital axis vector analysis
Polyanion species
C\(\_\)\(\_\) species, 99–103
dianion, 99–103
trianion, 99–103
Polyaromatic carbon molecules, 199
Polycrystalline sample, magnetic susceptibility measurements, 102
Polycyclic aromatic carbon (PAC) compound, 205, 206, 225, 226
σ-bonded transition metal complexes, 205–206
colloidal metal catalysis, 226
metal-PAC complex synthesis cluster complexes, 217–218
η¹ complexes, 207–213
metallacycle complexes, 214–217
metal-PAC reactions
metallacycle reductive elimination and cycloadditions, 219–223
metal migrations, 218–219
reactions at PAC, 223–225
Polycyclic aromatic hydrocarbons (PAHs), 2, 165, 179, 207, 217, 261
anions of, 63
bowl-shaped and basket-shaped, synthesis
cyclopentaindenotriphenylenes, 45
5-(2,6-dibromophenyl)-10-(1,1-dimethylpropyl)-11H-benzo[b]fluorene, 44
via palladium-catalyzed intramolecular arylation reactions, 44
carbanions, 64
with corannulene subunits, synthetic strategy, 14–15
curved PAHs, classification by Hopf, 63
POAV angles, 45, 46
twisted, 2
Polymer-like substance, 152
Polyrotaxanes, 343
Potassium cations, 103
Potassium tert-butoxide, 42
Potential clips with dibenzocyclooctadiene
tethers, 30–33
Princers, syn geometry, 1
Propargylic alcohol, 42
Pt(P(Et)3)2(2,2′-biphenyldiy)alkyne cycloaddition reactions, 222
Pulsed-gradient spin echo (PGSE), 67
Pulsed-gradient stimulated echo (PGStE) technique, 75
Pyramidalization, 45, 81, 88–90
Pyrenophane chemistry, 384–387
cycloaddition reactions of [n](2,7)pyrenophanes, 385
[n](2,7)pyrenophanes, unusual chemistry, 386
reduction of [n](2,7)pyrenophanes, 386
Quantum mechanical calculations, of carbanions, 67
Quinone, 16
Radical ion species, of corannulene derivatives, 106–107
experimental ESR spectra, 107
Raman bands, 285, 286
Raman spectra, 285
data, 139
Reductive aromatization reaction, 300
Retro–Claisen condensation, 49
Ring-closing metathesis (RCM) reaction, 190
Ring enlargement metathesis (REM), 264
construction system, 268
synthesis of aromatic belts, 264–279
ROM-RCM reactions, 195
Ru-catalyzed tandem ring-opening metathesis (ROM), 190
[Ru(Cp²)₂(μ²-η⁶:η⁶-C₂₀H₁₀)]²⁺, molecular structure, 160
Ruthenium-catalyzed isomerization, 241
Saponification, 49
Schmittel cyclization reactions, 41
Scott’s approach, 283
Selected ion flowtube (SIFT) apparatus, 158
Self-consistent field (SCF), 139
Semibuckminsterfullerenes, 8
nonpyrolitic synthesis of, 10
Sila–Friedel–Crafts reaction, 196
Silver complex, 323, 324
of picotube, 274
by reaction with AgClO₄ or AgOTf, 321
of tetrabenzo[16]annulene, 322
Silver(I)-based extended networks, 160
Single-crystal X-ray diffraction, 158
Single-walled nanotubes (SWNTs), 237, 238, 278
Sodium bis(2-methoxyethoxy)aluminum hydride, 243
Sodium methoxide, 13
Solid-state magnetic properties, 103
Sonogashira coupling reaction, 314, 317
Spin-spin distance, 101
Square planar bis(1-naphthyl) complex, atropisomers, 213
Stephen’s reagent, 299
Steric hindrance, 103
cis-Stilbene derivative, 317
Stokes–Einstein equation, 67
Sumanenes, 48, 187
  benzylc anions, condensation, 193
  bowl-to-bowl inversion, 87, 191–193
  chiral sumanene synthesis, 195
  coordination study of
    bowl-to-bowl inversion of CpRu
    sumanene, 198–199
  chiral complex, 198
  concave-selective
    complexation, 197–198
  deprotonation and quench of, 86
  extended π conjugation, 193
  heterasumanenes synthesis
    heterasumanenes having heteroatom
    functionalities, 196–197
    trisilasumanene, 196
    trithiasumanene, 195–196
  materials application, 199–200
  naphthosumanenes synthesis, 194–195
  stepwise anion generation at benzylic
    positions, 191
  structure, 87, 187, 190–191
  synthesis, 49, 188–190
  trianion, 86–88
Superconductivity, 95
Supramolecular tweezer-fullerene
  complexes, 3
Suzuki–Miyaura coupling reaction, 194, 304
Suzuki reaction conditions, 298

TD-DFT calculations, 148
Tebbe reagent, 57
Tensile strengths, 236, 292. See also Carbon
  nanotubes (CNT)
  biological material, 237
  structural steel, 237
Terabenzocyclooctatetraene system, 21
Tetralydrofuran ring, 49
Tethered [2.2]metacyclophanedienes
  formation of dihydropyrenophanes,
  mechanism for, 376
Tethered [2.2] metacyclophanes, 368
  syn/anti-isomerism, 368
  pyrenophanes from, 370
  synthetic approach, 369
Tethered pyrenes, 371
  aromaticity, 372
Tetrabenzocyclooctatetraene tether, 30
1,2,5,6-Tetrabromocorannulene, 11
Tetrabutylammonium fluoride (TBAF),
  54–56, 317, 318, 330, 331
1,2,4,5-Tetracyanobenzene (TCNB), 334
Tetradehydrodianthracene (TDDA), 264
  acyclic and cyclic alkenes, 266–267
  [n]annulenes, 268
  cyclo dimerization, 272–273
  molecular construction scheme, 265–266
  properties, 264
  quinoid and benzenoid structures, 267
  quinoid double bonds, 264
  reactions, 264
  reactivity, 264
  ring enlargement metathesis (REM), 265, 269, 271
  structure, 268
  synthesis, 264, 267
Tetrahedral σ-radical, 98
Tetraindenocorannulene, 141
1,6,7,10-Tetramethylfluoranthenes, 11, 14
1,3,6,8-Tetramethylnaphthalene, 243
Tetraphenylcyclopentadienone, 382
Tetraphenylene chiral synthesis, 221
Thermochromism, 338, 339
Thermolysis
  possible access to target structure, 353
  for synthesizing tetraacetate, 353
  CPMAS 13C NMR spectra, 357
  EPR spectra of thermolysis
  product, 355
  MALDI mass spectrum, 354
  UV-visible spectrum in
    chloroform, 355
Thiocarbonyldiimidazole (TCDI), 316
Thionocarbonate, 316
Thionyl chloride, 42
Three-membered metallacycle, 215
Time-dependent density functional theory
  (TD-DFT), 146, 148
Time-resolved microwave conductivity
  (TRMC) method, 200
INDEX 413

-o-TMS-corannulenyl triflate, 14
π–π’ Transition energy, 148
Transition metals, 159
complexes, 157
Tribenzo[12]annulene, 319
Trichlorodecacyclene, 251
Trideuteriosumanene, 193
Triethylsilane, 42
Triflic anhydride, 14
Trifluoroacetic acid, 42
Trifluoromethyl-substituted benzoates, 163
Triisopropylsilyl trifluoromethanesulfonate, 54
-o-Trimethylsilylaryltriflates, synthesis, 13
2-Trimethylsilylcorannulenyltrifluoromethanesulfonate, 30
η⁶-Trindane metal complex, 189
Trinitrobenzene, 30
Triphenylmethane radical, 97
Tris(trimethylsilyl) sumanene, 192
Trithiasumanene, 195
sequential intramolecular
sila-Friedel–Crafts reaction, 196
synthesis, 196
X-ray structural analysis, 195, 196
Tweezers
with bowl-shaped pincers, 36
in haystack, 33–35
binding energies of supramolecular
dimers, 34, 35
classic approaches, 33–34
entropy and solvation effects, 35
MM2 structures and binding energies, 35
molecular mechanics (MM) methods, 34
new DFT methods with dispersion
interactions, 34

Twin corannulene
with corannulene pincers and barrelene
tether, 17
synthesis, 16

Unsaturated cyclophanes, 330
UV-visible Absorption, 148

van der Waals interactions, 141
van der Waals surface, 272
Variable-temperature 1H NMR
experiment, 192
Variable temperature (VT) NMR
spectroscopy, 66, 211
Verdazyl radical-substituted
corannulene, 108
VID reaction, 371
energetics, 371
pyrenophane synthesis using,
372–374
anti-[2.2](1,8)pyrenophane, 373
[2.2]cyclophanes of pyrene and benzene, 379–384
[n](2,7)pyrenophanes, 373–379
quantifying aromaticity, 372
valence isomerization, key issue, 371

Wacker oxidation, 246, 247
Wittig reactions, 262

X-ray crystallographic analysis, 190, 198
X-ray diffraction analysis, 162, 164, 170, 171, 176

Zeolite-templated carbon (ZTC), 95
Zero INDO (ZINDO), 146, 148