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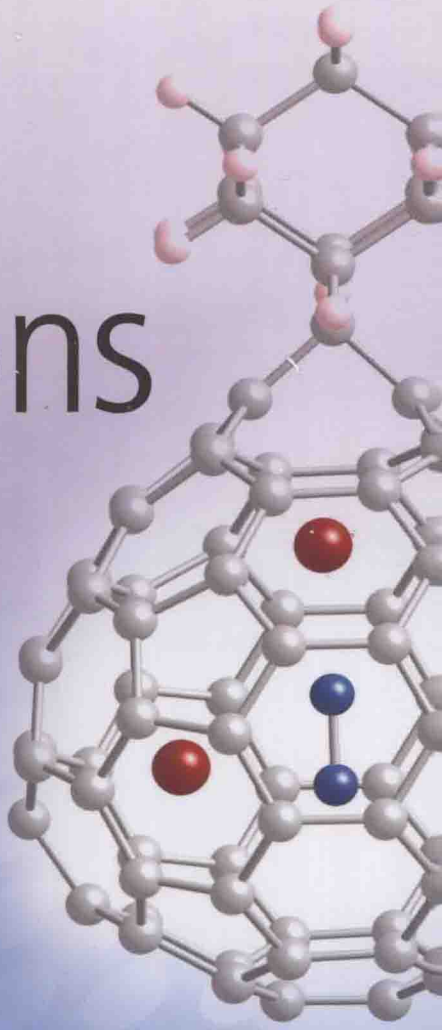
Chemistry of Nanocarbons



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Chemistry of Nanocarbons

We dedicate this monograph to the memory of R. Smalley and to the original discoverers Harry Kroto and Sumio Iijima

Preface

The first time I heard about the possibility of the existence of the molecule we now call buckminsterfullerene was at a lecture given by the late Prof. Orville Chapman in the mid 1980s, followed by the first disclosure by Kroto *et al.* in their *Nature* paper of 1985. In 1990, while visiting Robert Haddon at the AT&T Bell laboratories, I learnt that it had actually been synthesized, not by chemists but by physicists, referring, of course, to a preprint by W. Kraetschmer *et al*'s now famous 1990 *Nature* paper that was floating around the Labs. Since then, buckminsterfullerene has spawned an entire field of endeavor and this book tries to capture the most salient features of the novel molecular allotropes of carbon.

The chapters within this volume present the most up-to-date research on chemical aspects of nanometer sized forms of carbon. It therefore emphasizes the chemistry aspects of fullerenes, nanotubes and nanohorns. All modern chemical aspects are mentioned, including noncovalent interactions, supramolecular assembly, dendrimers, nanocomposites, chirality, nanodevices, host-guest interactions, endohedral fullerenes, magnetic resonance imaging, nanodiamond particles and graphene. The reader will be exposed to the most recent potential and actual applications of these remarkable allotropes of carbon in molecular electronics as well as medicine. The authors of the nineteen chapters are the current principal exponents of nano allotropes of carbon.

The subjects of this book would not be possible without the pioneering work of (in alphabetical order) Curl, Huffman, Iijima, Kraetschmer, Kroto and Smalley, and it is hoped that the book's contents will contribute to the lasting memory of these scientists.

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T. Akasaka, F. Wudl and S. Nagase gratefully acknowledge the support they received from their respective institutions during the process of this book's edition. We also thank the chapter authors for their prompt cooperation and help to produce this book that we believe will be an invaluable source of information to future researchers in the field.

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Abbreviations

ACCVD	alcohol catalytic chemical vapor deposition
AFM	antiferromagnetic
AFM	atomic force microscopy
AGNRs	armchair-edged graphene nanoribbons
AMI	Austin model 1
AMOs	antibonding molecular orbitals
ArcNTs	AP-grade single-walled carbon nanotubes
ATRP	atom transfer radical polymerization
BET	Brunauer, Emmett, and Teller
BIGCHAP	*N*,*N*-bis(3-D-gluconamidopropyl) cholamide
BMOs	bonding molecular orbitals
BODA	*bis-o*-diynyl arene
BSA	bovine serum albumin
BWF	Breit–Wigner–Fano
CAs	circumacenes
CAN	ammonium cerium(IV) nitrate
CaNCN	calcium cyanamide
CAPTEAR	chemically adjusting plasma temperature, energy, and reactivity
CD	circular dichroism
CIP	Cahn, Ingold, Prelog
CNG	carbon nanographene
CNOs	carbon nano onions
CNs	carbon nanotubes
CNTs	carbon nanotubes
COOH	carboxylic acid
CPE	constant potential electrolysis
CPPAs	cyclic [n]paraphenyleneacetylenes
CSCNTs	cup-stacked carbon nanotubes
CSP	chiral stationary phases
CT	charge transfer
CV	cyclic voltammetry
CVD	chemical vapor deposition
DABCO	1,4-diazabicyclo[2.2.2]octane
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DFT	density functional theory

DFT	discrete Fourier transform
DFT-GGA	density functional theory-generalized gradient-corrected approximation
DGU	density gradient ultracentrifugation
DLS	dynamic light scattering
DMA	dimethylacetamide
DMA	9,10-dimethylanthracene
DMAc	dimethylacetamide
DMAP	dimethylaminopyridine
DMF	dimethylformamide
DMRG	density matrix renormalization group
DMSO	dimethylsulfoxide
DN	detonation nanodiamond
DNA	deoxyribonucleic acid
DOS	density of states
DPV	differential pulse voltammetry
dsDNA	double-strand DNA
DTAB	dodecyltrimethylammonium bromide
DWNT	double wall carbon nanotube
ECF	extracellular fluid space
EMAPS	electromagnetically accelerated plasma spraying
EMFs	endohedral metallofullerenes
EPR	electron paramagnetic resonance
ES	electrostatic
exTTFs	π-extended tetrathiafulvalenes
FAD	flavine adenine dinucleotide cofactor
FET	field-effect transistors
FFF	field flow fractionation
FM	ferromagnetic
FTIR	Fourier transform infrared spectroscopy
GBL	γ-butyrolactone
G/D	graphite/defect
GGA	generalized-gradient approximation
GIAO	gauge-including atomic orbital
GlcNAc	*N*-acetyl-D-glucosamine
GNR	graphene nanoribbon
GOx	glucose oxidase
GPC	gel permeation chromatography
HEM	high energy mode
HiPco	high-pressure CO conversion
HMQC	hetero multiple bond correlation
HOMO	highest occupied molecular orbital

HOPG	highly oriented pyrolitic graphite
HPHT	high pressure high temperature
HPLC	high performance liquid chromatography
HRTEM	high-resolution transmission electron microscope
HSVM	high-speed vibration milling
HTAB	hexadecyltrimethylammonium bromide
IEC	ion exchange chromatography
IPCE	internal photon-to-current efficiency
IPR	isolated pentagon rule
IR	infrared
ITO	indium tin oxide
IUPAC	International Union of Pure and Applied Chemistry
LB	Langmuir-Blodgett
LCAO	linear combination of atomic orbitals
LDA	local density approximation
LDS	lithium, dodecyl sulfate
LPC	lysophosphatidylcholine
LPG	lysophosphatidylglycerol
LUMO	lowest unoccupied molecular orbital
MALDI-TOF-MS	matrix assisted laser desorption ionization time-of-flight mass spectrometry
MCPBA	*m*-chloroperbenzoic acid
MEM	maximum entropy method
MeOH	methanol
MNDO	modified neglect of differential overlap
MPWB1K	hybrid meta DFT method for kinetics
MRA	magnetic resonance angiography
MRI	magnetic resonance imaging
MWCNTs	multi-walled carbon nanotubes
MWNTs	multi-walled carbon nanotubes
NFE	nearly free electron
NHE	normal hydrogen electrode
NICS	nucleus independent chemical shifts
NIR	near-IR
NM	nonmagnetic
NMP	*N*-methyl-2-pyrrolidone
NMR	nuclear magnetic resonance
NMRD	nuclear magnetic relaxation dispersion
NSB	nonspecific binding
NW	nanowire

OC	*o*-carboxymethyl chitosan
ODA	octadecylamine
ODCB	*o*-dichlorobenzene
OITB	orbital interactions through bonds
OPV	oligophenylenevinylene
PABS	poly(*m*-aminobenzenesulfonic acid)
PAH	polycyclic aromatic hydrocarbons
PAMAM	poly(amido amine)
PAmPV	poly{(5-alkoxy-m-phenylenevinylene)-co-[(2,5-dioctyloxy-p-phenylene)-vinylene]}
PArcNTs	oxidized single-walled carbon nanotubes
PAs	periacenes
PBS	phosphate buffered saline
PCBM	methanofullerene phenyl-C_{61}-butyric acid methyl ester
PDDA	poly(diallyl dimethylammonium) chloride
PEO	polyethylene oxide
PEO-PDEM	poly(ethylene oxide)-*b*-poly[2-(*N*,*N*-dimethylamino)-ethyl methacrylate]
PEO-PDMS-PEO	poly(ethyleneoxide)-*b*-poly(dimethylsiloxane)-*b*-poly-(ethylene oxide)
PEO-PPO	poly(ethylene oxide)-*b*-poly(propylene oxide)
PEO-PPO-PEO	poly(ethylene oxide)-*b*-poly(propylene oxide)-*b*-poly-(ethylene oxide)
PDMS	poly(dimethylsiloxane)
PFG-NMR	pulsed-field gradient nuclear magnetic resonance
PFH-A	poly[(9,9-dihexylfluorenyl-2,7-diyl)-*co*-(9,19-anthracence)]
PFO	poly(9,9-dioctylfluorenyl-2,7-diyl
PFO-BT	poly[9,9-dioctylfluorenyl-2,7-diyl)-co-1,4-benzo-{2,1′-3}-thiadiazole)]
PhCN	benzonitrile
PL	photoluminescence
PLE	photoluminescence excitation
PLV	pulsed-laser vaporization
PMMA	poly(methylmethacrylate)
PMMA-PEO	poly(methylmethacrylate)-*b*-poly(ethylene oxide)
PmPV	poly-*m*-phenylenevinylene
PNIPAM	poly(N-isopropylacrylamide)
POAV	p-orbital axis vector analysis
PPEs	poly(aryleneethynylene)s
PPV	*p*-phenylenevinylene
PS-P4VP	polystyrene-*b*-poly(4-vinylpyridine)
PS-PBA	polystyrene-*b*-poly(*tert*-butyl acrylate)
PS-PBD-PS	polystyrene-*b*-polybutadiene-*b*-polystyrene
PS-PEO	polystyrene-*b*-poly(ethylene oxide)
PS-PI	polystyrene-*b*-polyisoprene

PS-PMAA	polystyrene-*b*-poly(methacrylic acid)
PS-PSCI	polystyrene-*b*-poly[sodium(2-sulfamate-3-carboxylate)isoprene]
PSA	prostate specific antigen
PSS^{n-}	poly(sodium 4-styrenesulfonate)
PTCDA	perylene tetracarboxylic dianhydride
$PVBTA^{n+}$	poly((vinylbenzyl)trimethylammonium chloride)
PVP	poly(4-vinylpyridine)
PZC	point of zero charge
QCM	quartz crystal microbalance
RBM	radial breathing mode
RDX	cyclotrimethylenetrinitramine
RNA	ribonucleic acid
SAM	self-assembled monolayers
SANS	small angle neutron scattering
SBM	Solomon-Bloembergen-Morgan
SC	sodium cholate
SCC-DFTB	self-consistent charges density functional theory of tight binding
SCCNT	stacked-cup carbon nanotubes
SDBS	sodium dodecyl benzene sulfonate
SDC	sodium deoxycholate
SDS	sodium dodecyl sulfate
SEC	size exclusion chromatography
SEM	scanning electron microscopy
SGC	sodium glycocholate
SiPc	silicon-phthalocyanine
SNBD	single-nano buckydiamond
SpA	staphylococcal protein A
ssDNA	single-strand DNA
STC	sodium taurocholate
STDC	sodium taurodeoxycholate
SWCNTs	single-walled carbon nanotubes
SWNHox	hole-opened single-walled nanohorns
SWNHs	single-walled nanohorns
SWNTs	single-walled carbon nanotubes
SWNs	single-walled carbon nanotubes
TDAE	tetrakis(dimethylamino)ethylene
TEM	transmission electron microscopic
TFA	trifluoroacetic acid
TGA	thermogravimetric analysis
THF	tetrahydrofuran
THPP	5,10,15,20-tetrakis(hexadecyloxyphenyl)-21*H*,23*H*-porphyrin
TMPD	*N*,*N*,*N*′,*N*′-tetramethyl-*p*-phenylenediamine

TMWCNTs	thin multi-walled carbon nanotubes
TNT	trinitrotoluene
TNTs	trimetallic nitride template endohedral fullerenes
TTAP	tetradecyl trimethyl ammonium bromide
TTF	tetrathiafulvalene
UDD	ultra-dispersed diamond
US	ultra-short
UV-vis	ultraviolet-visible
VDW	Van der Waals
VTMWCNTs	very thin multi-walled carbon nanotubes
VT-NMR	variable temperature nuclear magnetic resonance
XPS	X-ray photoelectron spectrum
XRD	X-ray diffraction
ZGNR	zigzag-edged graphene nanoribbon
ZINDO	*Zerner* Intermediate Neglect of Differential Overlap
ZnNc	zinc naphthalocyanine
ZnP	zinc tetraphenylporphyrin
ZnPP	zinc protoporphyrin

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