

CONTENTS

Preface.....	i
P.V. Kamat, D.M. Guld, and K.M. Kadish	

I. Electrochemistry and ESR

Overview: Electrochemical and ESR Spectroscopy Studies of Fullerenes and Their Derivatives.....	2
F. D'Souza	
Recent Advances in Electroactive Organofullerenes.....	4
N. Martin, L. Sanchez, B. Illescas, J.L. Segura, M.A. Herranz, and D.M. Guld	
Light-Induced Formation of C₆₀ Radical Adducts as Studied with Fourier Transform EPR.....	18
R. Groß and K.-P. Dinse	
S_{N1} Reactions of t-BuC₆₀⁻ with Sterically Hindered Alkyl Halides and Organic Cations.....	28
S. Fukuzumi, T. Hirasaka, T. Suenobu, X. Gao, and K.M. Kadish	
Electrochemical Behaviour of Hydrofullerene C₆₀H₃₆.....	38
A.S. Lobach and V.V. Strelets	
Electrochemical Properties of MC₆₀ (M = Pd, Pt) Covered Electrodes.....	47
A. de Bettencourt-Dias, K. Winkler, A. Hayashi, and A.L. Balch	
Electrogeneration and Characterization of a (C₆H₅CH₂)₂C₇₀ Mixture.....	59
K.M. Kadish, X. Gao, O. Gorelik, E. Van Caemelbecke, T. Suenobu, and S. Fukuzumi	
Electrochemistry of Adducts of 2-Cyano-2-Propyl Radicals to C₆₀.....	71
W.T. Ford, T. Nishioka, F. Qiu, F. D'Souza, J.-P. Choi, W. Kutner, and K. Noworyta	
New Heterobimetallic Palladium-[60]Fullerene Complex with Ferrocenyl-Phosphine Ligand.....	76
T.V. Magdesieva, V.V. Bashilov, D.N. Kravchuk, P.V. Petrovskii, A.G. Ginzburg, V.I. Sokolov, and K.P. Butin	
Proton-Induced Redox Tuning and Orientation of 2-(n-Alkyl)fullero-pyrrolidines in Langmuir Films.....	84
W. Kutner, K. Noworyta, M.S. Rahman, G.R. Deviprasad, and F. D'Souza	

Electrosynthesis and Characterization of $(C_6H_5CH_2)_4C_{60}$ Isomers.....	92
K.M. Kadish, X. Gao, E. Van Caemelbecke, T. Suenobu, and S. Fukuzumi	

II. Fullerene Functionalization and Biochemical / Pharmaceutical

Fullerene Functionalization.....	116
M. Maggini	
New Modified Fullerenes from Cycloaddition Reactions: Fullerotriazoline-TTF Dyads.....	119
S. Gonzalez, N. Martin, D.M. Guldi, A. Anton, J. Garin, and J. Orduna	
Synthesis, Chiroptical Properties and Electrochemistry of Bis-[di(alkoxycarbonyl)methano] [60]Fullerenes.....	127
R. Kessinger, C. Thilgen, F. Diederich, and L. Echegoyen	
Modulating the Electronic Properties of Fullerene Derivatives.....	139
M. Carano, P. Ceroni, F. Paolucci, S. Roffia, T. Da Ros, K. Kordatos, and M. Prato	
Formation of Fullerenes by Cyclization of Three-Dimensional Macroyclic Polyynes.....	146
Y. Tobe, H. Nakanishi, N. Nakagawa, and R. Furukawa	
Quantum Chemistry Study of Chemical Functionalization Reactions of Fullerenes and Carbon Nanotubes.....	153
R.L. Jaffe	
Methylation of [60]- and [70] Fullerene.....	163
H. Al-Matar and R. Taylor	
Formation and Characterization of a New Fullerene Dimer: $C_{121}O$.....	174
N. Dragoe, K. Nakahara, H. Shimotani, S. Tanibayashi, L. Xiao, and K. Kitazawa	
The First Structurally Characterized Homofullerene: 7,8-Dichloromethano-homo[70]fullerene.....	180
A.F. Kiely, R.C. Haddon, M.S. Meier, J.P. Selegue, C.P. Brock, B.O. Patrick, G.-W. Wang, and Y. Chen	
Isolation and Characterisation of Forty-Eight Fluorinated Derivatives of [70]Fullerene: The Ultimate HPLC Separation.....	188
R. Taylor, A.K. Abdul-Sada, O.V. Boltalina, and J.M. Street	
[60]Fullerene-Containing Thermotropic Liquid Crystals: New Anisotropic Materials	201
R. Deschenaux	

Synthesis and Photophysical Properties of Novel Fullerene Derivatives as Model Compounds for Bulk-Heterojunction PV Cells.....	206
P.A. van Hal, B.M.W. Langeveld-Voss, E. Peeters, R.A.J. Janssen, J. Knol, and J.C. Hummelen	
Enhancement of the Photoconductivity from the PPV/C₆₀ Composite Film.....	212
G. Ma, J. Qian, and S. Qian	
Singlet Oxygen Production of a Fulleropyrrolidine Chemically Bonded to Silica Gel.....	220
M. Bonchio, M. Maggini, E. Menna, G. Scorrano, L. Garlaschelli, A. Giacometti, F. Paolucci, F. Gasparrini, D. Misiti, and C. Villani	
Synthesis and Photophysical Properties of a Novel Parachute-Shaped C₆₀-Porphyrin Dyad.....	225
P. Cheng, S.R. Wilson, D.I. Schuster, S. Pyo, L. Echegoyen, R. Williams, G. Klihm, S.E. Braslavsky, and A. Holzwarth	
Clathrates of C₆₀ with Some n-Hydrocarbons.....	231
I.V. Arkhangelskii, E.V. Skokan, Y.A. Velikodnyi, N.B. Tamm, N.V. Chelovskaya, D.E. Izotov, A.V. Novikov, L.N. Sidorov, and V.I. Privalov	
Hexa(sulfobutyl)fullerene-Induced Photodynamic Effect on Tumors in Vivo and Toxicity Study in Rats.....	238
Y. Chi, T. Canteenwala, H.H.C. Chen, B.-J. Chen, M. Canteenwala, and L. Y. Chiang	
Metallofullerene Sample Analysis by Mass Spectrometry (LD-TOF MS), Neutron-Activation Analysis (NAA) and Inductively-Coupled-Plasma Atomic Emission Spectroscopy (ICP-AE).....	250
D.W. Cagle, J.M. Alford, and L.J. Wilson	
A Molecular Dynamics Study of HIV-1 Protease Complexes with C₆₀ and Fullerene-Based Anti-Viral Agents.....	256
H. Mi, M.E. Tuckerman, D.I. Schuster, and S.R. Wilson	

III. Photophysics and Photochemistry

Photochemistry and Photophysics of Fullerenes and Functionalized Fullerene Materials.....	271
D.M. Guldi and K.-P. Dinse	
Fullerenes as Photoinduced Electron Acceptors: From Photophysics to Photovoltaics.....	279
N.S. Sariciftci	

Acceleration of Photoinduced Electron Transfer in Porphyrin-Linked Fullerene.....	286
H. Imahori, K. Tamaki, H. Yamada, Y. Sakata, Y. Nishimura, I. Yamazaki, A. Shimomura, and T. Okada	
Photoinduced Charge Separation in Clusters of Fullerene-Aniline Dyads.....	296
V. Biju, K. George Thomas, M.V. George, D.M. Guldì, and P.V. Kamat	
Radical Ion Pairs in Sexithiophene/Fullerene Blends Studied by Transient EPR Spectroscopy.....	304
L. Pasimeni, M. Ruzzi, M. Prato, T. Da Ros, G. Barbarella, and M. Zambianchi	
Rate Constants of Reactions with 2-Cyano-2-Propyl Radical and Triplet State Lifetimes of Low Molar Mass and Polymeric Substituted [60]Fullerenes.....	315
D.M. Guldì, W.T. Ford, and T. Nishioka	
Photoinduced Electron Transfer of Fullerenes with Organic Donors and Acceptor in Solution.....	319
O. Ito and M. Fujitsuka	
Multiple Electron Transfers in Fullerene Derivatives ? A Study of (Donor)_N-[60]Fullerene Redox Molecular Systems.....	331
W. Huang, Z. Gao, R. Guduru, J.E. Mullins, and Y.-P. Sun	
New Concepts for Improving Charge Separation in Fullerene Containing Systems.....	341
D.M. Guldì, M. Prato, M. Maggini, and N. Martin	
Photoalkylation of C₇₀ with 4-Alkyl NADH Analogs via Photoinduced Electron Transfer.....	346
S. Fukuzumi, T. Hirasaka, T. Suenobu, O. Ito, M. Fujitsuka, X. Gao, and K.M. Kadish	
The Photophysical Properties of Azafullerenes C₅₉HN and its Dimer (C₅₉N)₂.....	359
B. Ma, A. Weitz, and F. Wudl	
Singlet State and Triplet State Properties of Pseudo-Dihydro Derivatives of C₇₀.....	368
S. Foley, M.N. Berberan-Santos, A. Fedorov, D.J. McGarvey, C. Santos, and B. Gigante	
Photophysics of Fullerene Derivatives.....	381
A.F. Benedetto, S.M. Bachilo, and R.B. Weisman	
Femtosecond Nonlinear Optical Response of the C₆₀(CH₃)_x(PAN)_x Copolymer.....	390
S. Qian, G. Ma, J. Qian, Y. Chen, R. Cai, L. Lin, W. Qian, and Y. Zou	

Optical Limiting of Fullerenes. Why are the Results so Different in Solution vs in Solid Matrix.....	398
Y.-P. Sun and J.E. Riggs	
Photophysical and Photochemical Properties of Pyrrolidinofullerenes.....	411
C. Luo, D.M. Guldi, M. Fujitsuka, O. Ito, T. Da Ros, and M. Prato	
Photochemistry of Fullerenes in the Near Infrared.....	424
L. Juha, B. Ehrenberg, S. Couris, E. Koudoumas, F.P. Boody, V. Hamplova, Z. Pokorna, A. Müllerova, and M. Pavel	
Photoluminescence Study of the Star-Like C₆₀(CH₃)(PAN)₃ Copolymer.....	438
G. Ma, S. Qian, Y. Mo, Y. Chen, R. Cai, and X. Ye	
Layered Materials by Electron Transfer Induced Deposition of Fullerene C₆₀.....	444
Y.A. Dubitsky, O.N. Efimov, Y.V. Korneenkov, E.P. Krinichnaya, A.S. Lobach, A.P. Moravskii, V.V. Strelets, L.I. Tkachenko, and A. Zaopo	

IV. Thermodynamics and Mass Spectroscopy

Mass Spectrometry and Thermodynamics of Fullerenes.....	451
O.V. Boltalina and G. Gigli	
Production of Fullerenes from Various Carbon Materials by Means of JxB Arc Jet Reactors.....	453
T. Mieno and A. Sakurai	
Fluorination of Aza[60]Fullerene.....	462
O.V. Boltalina, T. Drewello, A. Hirsch, T.J.D. Jörgensen, V.U. Markov, U. Reuther, and R. Taylor	
Vapour Pressure Measurements on Fullerenes and Fluorofullerenes.....	472
G. Gigli	
Ion-Molecular Equilibria Between Fullerenes and Their Difluorides in the Gas Phase.....	484
L.N. Sidorov, O.V. Boltalina, A. Ya Borschevsky, and I.N. Ioffe	
Solid Solvates of C₆₀ with Halobenzenes.....	494
A.L. Mirakyan, M.V. Korobov, N.V. Avramenko, and R.S. Ruoff	
Controlled by Energy Interactions of Free Electrons with Molecules of Hydrogenated Fullerenes.....	499
Y.V. Vasil'ev, R.R. Abzalimov, A.S. Lobach, S.K. Nasibullaev, Y.M. Shul'ga, and V.A. Mazunov	

Thermodynamic Properties of Hydrofullerene C₆₀H₃₆ in the Range of 5-340 K.....506
B.V. Lebedev, T.A. Bykova, and A.S. Lobach

DSC and X-Ray Diffraction Study of the Fluorofullerene Solvates.....516
P.A. Troshin, Y.A. Makeev, N.V. Chelovskaya, Y.L. Slovokhotov, O.V.
Boltalina, and L.N. Sidorov

**C₆₀ Fluorination by Molecular Fluorine: Routes of Selective Synthesis of
Fluorofullerenes.....531**
N.S. Chilingarov, A.V. Nikitin, J.V. Rau, F.M. Spiridonov, I.V. Golyshevskij,
A.V. Kepman, and L.N. Sidorov

**Solid State Fluorination of Fullerenes with Distillation of the Volatile
Products.....540**
A.Y. Borshchevsky, O.V. Boltalina, and L.N. Sidorov

V. Nanotubes and Nanocarbons

**Realization and Observation of the Reversible and Irreversible Radial
Deformation of Carbon Nanotubes by Tapping Mode Atomic Force
Microscopy.....552**
M. Yu, R.S. Ruoff, T. Kowalewski, M.J. Dyer, J.R. Von Ehr, B. Faircloth, and
R.R. Krchnavek

Cesium Induced Graphitization of Amorphous Carbons.....558
S. Subramoney, H. C. Foley, and J.G. Chen

**Recent Progress in the Production of Multi-Wall Carbon Nanotubes Using
Various Supported Cobalt Catalysts.....566**
P. Piedigrosso, Z. Konya, J.-F. Colomer, A. Fonseca, K. Hernadi, G. Van
Tendeloo, and J.B. Nagy

Computer Simulation of H₂ Encaging into Carbon Nanotube.....580
V.A. Eltekov

VI. Solid States Physics

**Raman Line Shapes in A₃C₆₀ (A=K, Rb): Effects of Orientational Disorder
on Phonon Spectra.....588**
O. Gunnarsson and J.E. Han

**Critical Current Density and Evidence for Bulk Superconductivity in
Fullerene Superconductors.....597**
V. Buntar, C. Krutzler, F.M. Sauerzopf, H.W. Weber, M. Haluska, and H.
Kuzmany

Electronic Structure of Polymerized Fullerene.....	608
L.G. Bulusheva, V.V. Belavin, A.V. Okotrub, and D. Tomanek	
Molecular Complexes of Fullerenes C₆₀ and C₇₀ with Organic Donors.....	615
R.N. Lyubovskaya and D.V. Konarev	
Electrical Properties of the Rhombohedral C₆₀ Polymers.....	628
T.L. Makarova, T. Wagberg, B. Sundqvist, V. Agafonov, V.A. Davydov, A.V. Rakhmanina, and L.S. Kashevarova	
A Molecular Dynamics Study on the Formation of Metallofullerene.....	640
Y. Yamaguchi and S. Maruyama	
Interaction of Platinum Fulleride C₆₀Pt with Deuterium: IR and X-ray Photoelectron Studies.....	647
N.F. Goldshleger, B.P. Tarasov, Y.M. Shul'ga, O.S. Roschupkina, A.A. Perov, and A.P. Moravsky	
Multiaxial Reorientation of C₆₀ and Phase Transition in Fullerite: Theory and NMR Experiments.....	653
D.E. Isotov, V.P. Tarasov, V.I. Privalov, E.V. Skokan, I.V. Arkhangel'skii, Y.A. Velikodnyi, and L.N. Sidorov	
Spectroscopic Properties of Individual Pressure-Polymerized Phases of C₆₀.....	665
V.A. Davydov, L.S. Kashevarova, A.V. Rakhmanina, V. Agafonov, H. Allouchi, R. Ceolin, V.M. Senyavin, G. Sagon, and H. Szwarc	

VII. Theory

Seattle Theoretical Session: An Introductory Survey.....	677
E. Osawa and Z. Slanina	
Computing Less-Rounded Cages: C₃₆ Non-IPR Fullerenes and Quasi-Fullerenes.....	682
Z. Slanina, X. Zhao, and E. Osawa	
Models of Fullerene Reactivity.....	693
P.W. Fowler, K.M. Rogers, J.P.B. Sandall, K.R. Somers, A. Troisi, and D.B. Redmond	
A Catalytic Mechanism of Fullerene Formation in Coal.....	701
E. Osawa, Z. Slanina, M. Ozawa, X. Zhao, and M. Saunders	
Evaluation of the Relative Stabilities of the IPR and Non-IPR Structures of C₈₄.....	711
X. Zhao, K.H. Lee, Z. Slanina, and E. Osawa	

**Fullerenes with Metal Overlayer: Calculations on C_mM_n ($m = 60, 70$; $n = 12$,
20/25, 32/37; $M = Be, Mg, Al$).....723
C. Miyajima, X. Zhao, Z. Slanina, L. Adamowicz, and E. Osawa**

**$C_{60}(NO_2)_2$, $C_{60}(NO_2)_4$, and $C_{60}(NO_2)_6$: Computed Energetics and Structures.....734
Z. Slanina, X. Zhao, F. Uhlik, L.Y. Chiang, and E. Osawa**

VIII. Endofullerenes

**Overview of Endohedral Fullerene Session.....746
T. Akasaka**

**Efficient Production of Endohedral Metallo-Fullerenes in Gravitation-Free
Arc Discharge by Means of a Vertical-Swing-Tower.....749
T. Mieno**

**Spin Chemistry of Metallofullerenes.....756
T. Kato, K. Yamamoto, S. Okubo, and T. Akasaka**

**Electrochemical Study on Electronic Structure of Mono-Lanthanofullerenes
of $La@C_n$ ($n = 82, 86$ and 90).....761
K. Yamamoto**

**Isolation and Characterization of a $Pr@C_{82}$ Isomer.....771
T. Akasaka, S. Okubo, T. Wakahara, K. Yamamoto, T. Kato, T. Suzuki, S.
Nagase, and K. Kobayashi**

**Radiolabelled Endohedral Fullerenes by Nuclear Recoil Implosion.....779
T. Braun and H. Rausch**

**Are IPR-Satisfying Structures Most Stable for $Sc_3@C_{82}$ and $Sc_4@C_{82}$?.....787
K. Kobayashi, Y. Sano, and S. Nagase**

**Endohedral Metallofullerenes Based on Some Missing Fullerenes.....795
C.-R. Wang, T.J.S. Dennis, Y. Itho, T. Ogawa, and H. Shinohara**

**EPR Investigation of Atoms in Fullerene Traps.....806
K.-P. Dinse, H. Käß, N. Weiden, and C. Knapp**

**Free Internal Translation and Thermodynamic Properties of $He@C_{60}$ 816
Z. Slanina, F. Uhlik, and E. Osawa**

Author Index.....822

Key Word List827