

20th International Symposium on Radical Ion Reactivity (ISRIR 2006)
Villa Mondragone (Rome - Italy) July 2-6 2006

PROGRAM

Scientific Sessions Villa Mondragone – Sala degli Svizzeri
Poster Session Villa Mondragone – Portico del Vasanzio

Sunday, July 2

12.00-16.00 **Registration** (Hotel Villa Vecchia)

16.30-16.50 **Opening Remarks**

Chair: Enrico Baciocchi

16.50-17.40 **IL1 Helmut Schwarz**
From Bare FeO⁺ to Cytochrome P-450: New Insight in the Intriguing Mechanisms of C-H Bond Oxygenation

17.40-18.05 **IL2 Michael Schmittel**
How Radical Ion Chemistry Can Contribute to Lab-on-Microchip Technologies!

18.05-18.55 **IL3 Bronislaw Marciniak**
Reactive Intermediates in the Photo-oxidation of Sulfur-Containing Organic Compounds

20.00 **Welcome Cocktail**

20.45 **Dinner**

Monday, July 3

Chair: Jean-Michel Savéant

9.00-9.50 **IL4 Shunichi Fukuzumi**
A Variety of Binding Modes of Metal Ions with Radical Ions and Applications to Regulation of Electron Transfer

9.50-10.40 **IL5 Martin Newcomb**
Radical Cations from Radical Heterolysis Reactions

10.40-11.00 **Coffee Break**

Chair: Henry J. Shine

- 11.00-11.50 **IL6** **Jun-ichi Yoshida**
Radical/Radical Cation/Cation Crossover
- 11.50-12.10 **OL1** **Olivier Poizat**
*Dynamics of Protonation of a Radical Anion "Super" Photobase
in Aqueous Solution*
- 12.10-12.30 **OL2** **Andrea Cuppoletti**
*Effect of α -Substitution on the Efficiency of Photo-Cleavage of 2-
Nitropiperonylcarbonates for In-situ High Density DNA
Microarrays Synthesis*
- 12.30-12.50 **OL3** **Kazuhiko Mizuno**
Stereocontrol in Photoinduced Electron Transfer Reactions
- 12.50-14.30 **Lunch**

Chair: Ana L. Moore

- 14.30-15.20 **IL7** **Arvi Rauk**
The Chemistry of Alzheimer's Disease (Theoretically)
- 15.20-16.10 **IL8** **Christian Schöneich**
*Oxidation Mechanisms of Methionine Important for β -Amyloid
Toxicity, Alzheimer's Disease, and the Characterization of
Protein Degradation Hot Spots*
- 16.10-16.30 **OL4** **Alexandra Yurkovskaya**
Time-Resolved CIDNP Study of Radical Reactions of Proteins
- 16.30-16.50 **Coffee Break**

Chair: Nazario Martín

- 16.50-17.40 **IL9** **Robert P. Hanzlik**
*Radical-Cations, Cyclopropanes and Heme Enzyme: Big
Surprises from Small Rings*
- 17.40-18.30 **IL10** **Ana L. Moore**
Bioinspired Energy Conversion Schemes
- 18.30-18.50 **OL5** **Itzhak Bilkis**
*Tautomerism of Radical Species Originated from Nucleic Acid
Bases*
- 20.30 **Dinner**
- 22.00-22.20 **SL** **Heinz D. Roth**
A Tribute to Stanislao Cannizzaro

Tuesday, July 4

Chair: Joseph P. Dinnocenzo

- 9.00-9.50 **IL11 Heinz D. Roth**
Intramolecular Nucleophilic Capture/Substitution of Radical Cations
- 9.50-10.40 **IL12 Tetsuro Majima**
Photosensitized One Electron Oxidation of DNA Towards Photodynamic Therapy
- 10.40-11.00 **Coffee Break**

Chair: Cynthia J. Burrows

- 11.00-11.50 **IL13 Flavio Maran**
Electron Transfer Through Peptides
- 11.50-12.15 **IL14 Krzysztof Bobrowski**
Sulfide Radical Cation Chemistry in Cyclic Dipeptides
- 12.15-12.35 **OL6 Marija Bonifačić**
Oxidation Mechanism of Aliphatic α -Amino Acids in Aqueous Solutions; Electron Transfer from Amino vs. Carboxylate Functional Group
- 12.35-12.55 **OL7 Cyrille Costentin**
Does Reductive Dechlorination by Vitamin B12 and Corrinoid-based Dehalogenases Follow an Electron Transfer Mechanism? Role of Protonation
- 12.55-14.30 **Lunch**

Chair: Shunichi Fukuzumi

- 14.30-15.20 **IL15 Dirk M. Guldi**
Multifunctional Molecular Carbon Materials - from Fullerenes to Carbon Nanotubes
- 15.20-16.10 **IL16 Nazario Martín**
Electron Transfer in Novel Molecular and Supramolecular Fullerene and Carbon Nanotube Ensembles
- 16.10-16.30 **OL8 Ortwin Brede**
If the Molecules are Dancing: Free Electron Transfer in Non-polar Media
- 16.30-16.50 **Coffee Break**
- 16.50-19.00 **Poster Session**
- 20.30 **Dinner**

Wednesday, July 5

Chair: Robert P. Hanzlik

9.00-9.50 **IL17 Joseph P. Dinnocenzo**
Mechanism of Excited State Quenching by High E_{ox} n-Electron Donors

9.50-10.40 **IL18 Miguel A. Miranda**
Novel Photocycloadditions and Photocycloreversions under Electron Transfer Conditions

10.40-11.00 **Coffee Break**

Chair: Steen Steenken

11.00-11.50 **IL19 Cynthia J. Burrows**
Chemistry and Biology of Oxopurine Radical Cations in DNA

11.50-12.40 **IL20 Jean Cadet**
Recent Aspects of the Radical Ion Chemistry of Purine and Pyrimidine Bases in Isolated and Cellular DNA

12.40-13.00 **OL9 M. Samy El-Shall**
Structure and Reactivity of Organic Radical Cations in the Gas Phase

13.00-14.30 **Lunch**

Chair: Glauco Tonachini

14.30-15.20 **IL21 Paul E. Floreancig**
New Applications of Oxidative Cleavage Reactions

15.20-15.50 **IL22 Hermenegildo Garcia**
Photochemistry in Ionic Liquids

15.50-16.10 **OL10 Luigi Lopez**
Reactivity of Aminium Hexachloroantimonate Salts

16.10-16.30 **OL11 Cedric W. McClelland**
Radical and Radical-Cation Mediated Cyclisation Reactions: A Computational Study

16.30-16.50 **Coffee Break**

Chair: Michael Schmittel

16.50-17.40 **IL23 Angelo Albini**
Persistency and Reactivity of Some Radical Ions

- 17.40-18.30 **IL24 Thomas Bally**
Recent Studies of Radical Ions under Stable Conditions
- 20.00 ***Dinner at the Wine Museum of Monteporzio***

Thursday, July 6

Chair: Hermenegildo Garcia

- 9.00-9.20 **OL12 Victor A. Bagryansky**
*Direct Detection of Organic Radical Ions and Study of their
Reactivity in Nanosecond Time Domain by Spin Chemistry
Techniques*
- 9.20-9.40 **OL13 Georg Gescheidt**
*Photophysical Investigations on Photoinitiators with Covalently
Linked Thioxanthone Sensitizer Moieties*
- 9.40-10.30 **IL25 Stephen F. Nelsen**
*Charge-Localized and Charge-Delocalized Organic Intervalence
Compounds*
- 10.30-10.50 ***Coffee Break***

Chair: Carlo Galli

- 10.50-11.40 **IL26 James M. Mayer**
*Concerted Proton-Electron Transfer in the Oxidation of Phenol-
Base Compounds to Distonic Phenoxyl Radicals*
- 11.40-12.30 **IL27 Jean-Michel Savéant**
*Electrochemical Approach to Concerted Proton-Electron
Transfers*
- 12.30-12.45 **Concluding Remarks**
- 12.45 ***Lunch***