**Prof.ssa Simonetta Fornarini Curriculum vitae** 15.02.2019

SSD CHIM/03

*Dipartimento di Chimica e Tecnologie del Farmaco*

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* **Education**
	+ 1971-1976 Università degli Studi di Roma ‘La Sapienza’, Faculty of Natural, Physical and Mathematical Sciences, Master’s degree in Chemistry (summa cum laude), 16th December 1976.
	+ 1966-1971 Liceo Classico T. Tasso in Roma. “Diploma di maturità classica” July 1971.

* **Post graduate work**
	+ 1978-1979 research assistantship at the University of California, Santa Cruz (USA), with the award of a Fulbright grant
	+ 1977-1978 research assistantship at the Laboratory of Physical Chemistry of the Italian National Committee for Nuclear Energy (CNEN).
	+ 1976-1977 teaching assistantship at the Università degli Studi di Roma ‘La Sapienza’
* **Professional and academic positions**
	+ 2000 to the present: professor of Chemistry (professore ordinario di Chimica Generale e Inorganica. CHIM/03), Università degli Studi di Roma ‘La Sapienza’, Faculty of Pharmacy and Medicine
	+ 1992-2000 associate professor of General and Inorganic Chemistry, Università degli Studi di Roma ‘La Sapienza’, Faculty of Pharmacy
	+ 1983-1992 researcher, Università degli Studi di Roma ‘La Sapienza’, Faculty of Pharmacy
	+ 1981-1983 research scientist at the Italian National Research Council (CNR), Institute of Nuclear Chemistry
* **Research appointments and awards**
	+ 1988, 1991-to the present, principal investigator of fundamental research proposals funded by the Università degli Studi di Roma ‘La Sapienza’ and by the Italian Ministry of University and Research (MIUR)
	+ 2005 to the present, principal investigator of research proposals funded by the European Union for access to the IR free electron laser beamline of the CLIO center (Centre Laser Infrarouge d’Orsay), France.
	+ 2014 and 2015, principal investigator of research proposals funded by public (national and EU) sources for access to the CIRCULARPOLARIZATION beamline of the Elettra laboratory, Trieste, Italy.
	+ 1998 to the present: director of the scientific committee in charge of the departmental FT-ICR mass spectrometer
	+ 1998 invited professor (research seminars) at the University of Colorado, Boulder. Invited lecturer at the University of Pennsylvania, the University of Minnesota and Purdue University
	+ 1995 visiting professor at the University of Colorado, Boulder as Fulbright scholar.
	+ 1985 and 1987 research appointments at the Institute of Nuclear Chemistry of the CNR
* **Major research interests**
* Reaction mechanisms: investigation of mechanisms of bioinorganic reactions by means of mass spectrometry, ions spectroscopy and theoretical computations. The research spans from kinetic studies to the construction of potential energy-surfaces for a given reaction system. The systems of interest include: (i) high-valent oxo-metal species at the core of oxygenase enzymes, (ii) nitrosyl complexes that are responsible for the biological activity of NO, (iii) the structural and functional consequence of post-translational modifications of amino acids and peptides, (iv) reactivity and structural issues regarding the activity of cisplatin antitumor drug.
* Fundamental properties of molecules: experimental and theoretical investigation of basic thermodynamic properties of molecules such as ionization energies, proton affinities, or bonding energies. Studies of complexation abilities of molecules and of their redox properties.
* IR spectroscopy and structural characterization of gaseous ions: investigation of intrinsic properties, structure and reactivity of naked ions in order to find structural clues and novel modes in chemical interactions and reactivity.
* Cooperating with many scientists from Italy (Nazzareno Re from the Università di Chieti, Paolo Tosi from Università di Trento, Susanna Piccirillo from Università di Roma Tor Vergata) as well as from abroad (Hans-Ullrich Siehl (Universität Ulm), Jean-Yves Salpin (Université d'Evry Val d'Essonne), Philippe Maitre (Université Paris Sud), James M. Mayer (University of Washington), Carme Rovira (Barcelona Science Park), Paul M. Mayer (University of Ottawa), Dietmar Kuck (Universität Bielefeld), Otto Dopfer (Technische Universität Berlin), Sam P. de Visser (University of Manchester).
* **Qualifications and professional experience**
	+ Expertise in mass spectrometry (MS): ion cyclotron resonance MS, different types of multipole systems, ion traps, selected ion flow tubes.
	+ Expertise in alternative means for studying gas phase ion chemistry, including radiolytic techniques and NMR analysis of neutrals from ion molecule reactions.
	+ Expertise in measurements with free-electron laser systems and table-top laser systems.
	+ More than 160 papers in peer-reviewed scientific journals (including reviews (2) and chapters (4)), Hirsch-index 31 (Scopus). Integrated Impact Factor > 800.
	+ Orcid ID: 000-002-6312-5738
	+ Invited lectures at International conferences (e. g. ESOR, ESOC, KISPOC, IMSC, IUPAC) and at Italian and foreign universities (in USA, Canada, Europe).
* **Refereeing**
* Referee for the following international journals: Angewandte Chemie International Edition; Journal of the American Chemical Society, Chemistry a European Journal, Inorganic Chemistry, ChemPhysChem, Chemical Communications, Journal of Physical Chemistry, Journal of Mass Spectrometry, International Journal of Mass Spectrometry, European Journal of Inorganic Chemistry, Journal of the American Society of Mass Spectrometry.
* Member of the editorial board of International Journal of Mass Spectrometry.
* Referee for several funding organizations (e. g. European Research Council, Italian Ministry of University and Research, University of Padova, Petroleum Research Fund USA, European Science Foundation, Portuguese Foundation for Science and Technology, Netherlands Organization for Scientific Research (NWO))
* **Teaching activity**

For the *Master degree in Pharmaceutical Chemistry and Technology* at the Università degli Studi di Roma ‘La Sapienza’:

* 1993-94 to the present“General and Inorganic Chemistry”
* 1992-93 “Stoichiometry”
* 1997-98 “Bioinorganic Chemistry”
* 1983-1992 ancillary stoichiometry course for “General and Inorganic Chemistry”

For the *Bachelor degree in Geological Sciences* at the Università degli Studi di Roma ‘La Sapienza’:

* 2013-14 “General and Inorganic Chemistry and Basics of Organic Chemistry”

For the *Master degree in Pharmaceutical Chemistry and Technology* at the Università di Chieti “G. D’Annunzio”:

* 1991-92, 1993-94, 1994-95 “General and Inorganic Chemistry”
* **Publications (2008-2018)**

64. Fabián G. Cantú Reinhard, Simonetta Fornarini, Maria Elisa Crestoni, Sam P. de Visser

**Hydrogen atom versus hydride transfer in cytochrome P450 oxidations: A combined mass spectrometry and computational study**

*Eur. J. Inorg. Chem.* (2018), 1854-1865.

63. Davide Corinti, Daniele Catone, Stefano Turchini, Flaminia Rondino, Maria Elisa Crestoni, Simonetta Fornarini

**Photoionization mass spectrometry of -phenylalkylamines: role of radical cation- interaction**

*J. Chem. Phys.* (2018), 148, 164307/1-8.

62. Anatoly P. Sobolev , Luisa Mannina, Donatella Capitani, Gabriella Sanzò , Cinzia Ingallina, Bruno Botta, Simonetta Fornarini, Maria Elisa Crestoni, Barbara Chiavarino, Simone Carradori, Marcello Locatelli, Anna Maria Giusti, Giovanna Simonetti, Giuliana Vinci, Raffaella Preti, Chiara Toniolo, Massimo Reverberi, Marzia Scarpari, Alessia Parroni, Lorena Abete, Fausta Natella, Antonella Di Sotto

**A multi-methodological approach in the study of Italian PDO "Cornetto di Pontecorvo" red sweet pepper**

*Food Chem.* (2018), 255, 120-131.

61. Davide Corinti, Barbara Gregori, Leonardo Guidoni, Debora Scuderi, Terry B. McMahon, Barbara Chiavarino, Simonetta Fornarini, Maria Elisa Crestoni

**Complexation of halide ions to tyrosine: role of non-covalent interactions evidenced by IRMPD spectroscopy**

*Phys. Chem. Chem. Phys.* (2018), 20, 4429-4441.

60. Roberto Paciotti, Davide Corinti, Alberto De Petris, Alessandra Ciavardini, Susanna Piccirillo, Cecilia Coletti, Nazzareno Re, Philippe Maitre, Bruno Bellina, Perdita Barran, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

**Cisplatin and transplatin interaction with methionine: bonding motifs assayed by vibrational spectroscopy in the isolated ionic complexes**

*Phys. Chem. Chem. Phys.(* 2017), **19**, 26697-26707.

59. Alessandra Ciavardini; Simonetta Fornarini; Antonella Dalla Cort, Susanna Piccirillo, Debora Scuderi, Enrico Bodo

**Experimental and Computational investigation of Salophen-Zn Gas Phase Complexes with Cations: Possible Cationic Interference in Anionic Recognition**

J. Phys. Chem. A (2017), 121, 7042-7050

58. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Debora Scuderi, Jean-Yves Salpin

**Undervalued N3-Coordination Revealed in the Cisplatin Complex with 2′-Deoxyadenosine-5′-Monophosphate by a Combined IRMPD and Theoretical Study**

*Inorg. Chem.* (2017), 56, 8793–8801

57. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

**Vibrational signatures of gaseous Meisenheimer complexes bonded at carbon and nitrogen**

 *Int. J. Mass Spectrom.* (2017), 418, 173-179.

56. Alessandra Ciavardini, Antonella Dalla Cort, Simonetta Fornarini, Debora Scuderi, Anna Giardini, Gianpiero Forte, Enrico Bodo, Susanna Piccirillo

**Adenosine monophosphate recognition by zinc–salophen complexes: IRMPD spectroscopy and quantum modeling study**

*J. Molecular Spectroscopy* (2017), 335, 108–116.

55. Davide Corinti, Cecilia Coletti, Nazzareno Re, Susanna Piccirillo, Marco Giampà, Maria Elisa Crestoni, S. Fornarini

**Hydrolysis of cis- and transplatin: structure and reactivity of the aqua complexes in a solvent free environment**

*RSC Adv.* (2017), 7, 15877 – 15884.

54. Davide Corinti, Alberto De Petris, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

**Cisplatin Primary Complex with L-Histidine Target Revealed by IRMPD Spectroscopy**

*ChemPhysChem* (2017), 18, 318-325.

53. Fabián G. Cantú Reinhard, Mala A. Sainna, Pranav Upadhayay, G. Alex Balan, Devesh Kumar, Simonetta Fornarini, Maria Elisa Crestoni, Sam P. de Visser

**A systematic account on aromatic hydroxylation by a cytochrome P450 model Compound I: A low-pressure mass spectrometry and computational study**

*Chem. Eur. J.* (2016), 22, 18608-18619.

52. Debora Scuderi, Enrico Bodo, Barbara Chiavarino, Simonetta Fornarini, Maria Elisa Crestoni

**Amino-acids oxidation: a combined study of cysteine oxo-forms by IRMPD spectroscopy and simulations**

*Chem. Eur. J.* (2016), 22, 17239-17250.

51. Markus Schütz, Aude Bouchet, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Otto

Dopfer

**Effects of Aromatic Fluorine Substitution on Protonated Neurotransmitters: The Case of 2-Phenylethylamine**

*Chem. Eur. J.* (2016), 22, 8124-8136.

50. Simonetta  Fornarini, Barbara Chiavarino, Davide Corinti, Luisa Mannina, Vincent Steinmetz, Maria Elisa Crestoni

**IRMPD signature of protonated pantothenic acid, a ubiquitous nutrient**

*Chemical Physics Letters*  (2016), 646, 162-167

49. Davide Corinti, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

**Cisplatin Binding to Biological Ligands Revealed at the Encounter Complex Level by IR Action Spectroscopy**

*Chem. Eur. J.* (2016), 22, 3794-3803.

48. Roberto Paciotti, Cecilia Coletti, Nazzareno Re, Debora Scuderi,Barbara Chiavarino, Simonetta Fornarini, Maria Elisa Crestoni

**Serine *O*-sulfation probed by IRMPD spectroscopy**

[*Phys. Chem. Chem. Phys.*](http://pubs.rsc.org/en/journals/journal/cp) (2015), **17**, 25891-25904.

47. Aude Bouchet,Markus Schütz,Barbara Chiavarino,Maria Elisa Crestoni,Simonetta Fornarini,Otto Dopfer

**Infrared spectrum and anharmonic calculations of the protonated neurotransmitter 2 phenylethylamine: Effects of dispersion and vibrational anharmonicity in the NH3+-π interaction**

[*Phys. Chem. Chem. Phys.*](http://pubs.rsc.org/en/journals/journal/cp) (2015), **17**, 25742-25754.

46. Rajeev K. Sinha, Debora Scuderi, Philippe Maitre, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

**Elusive Sulfurous Acid: Gas Phase Basicity and IR Signature of the Protonated Species**

*J. Phys. Chem. Lett.* (2015), *6*, 1605–1610

45. Maria Elisa Crestoni, Barbara Chiavarino, Simonetta Fornarini

**Nitrosyl-Heme and Anion-Arene Complexes: Structure, Reactivity and Spectroscopy**

*Pure and Applied Chemistry* (2015), 87, 379-390.

44. Chiavarino, Barbara; Crestoni, Maria Elisa; Fornarini, Simonetta; Scuderi, Debora; Salpin, Jean-Yves

**Interaction of cisplatin with dGMP : a combined IRMPD and theoretical study**

*Inorg. Chem.* (2015), 54, 3513-3522.

43. Alberto De Petris, Maria Elisa Crestoni, Adele Pirolli, Carme Rovira, Javier Iglesias-Fernández, Barbara Chiavarino, Rino Ragno, Simonetta Fornarini

**Binding of Azole Drugs to Heme: A Combined MS/MS and Computational Approach**

*Polyhedron* (2015), 90, 245-251.

42. Alberto De Petris, Barbara Chiavarino, Maria Elisa Crestoni, Cecilia Coletti, Nazzareno Re, Simonetta Fornarini

 **Exploring the Conformational Variability in the Heme b Propionic Acid Side Chains through the Effect of a Biological Probe: A Study on the Isolated Ions**

 *J. Phys. Chem. B* (2015), 119, 1919-1929.

41. Mala A Sainna, Suresh Kumar, Devesh Kumar, Simonetta Fornarini, Maria Elisa Crestoni, Samuel de Visser

[**A comprehensive test set of epoxidation rate constants by iron(IV)-oxo porphyrin cation radical complexes**](http://pubs.rsc.org/en/content/articlelanding/2014/sc/c4sc02717e)

Chemical Science (Chem. Sci.) (2015), **6**, 1516 – 1529.

40. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

 **Intrinsic Properties of Nitric Oxide Binding to Ferrous and Ferric Hemes**

 *Croatica Chemica Acta* (2014), 87, 307-314.

39. Barbara Gregori, Leonardo Guidoni, Barbara Chiavarino, Debora Scuderi, Edith Nicol, Gilles Frison, Simonetta Fornarini, Maria Elisa Crestoni

**Vibrational signatures of S-nitroso glutathione as gaseous, protonated species**

 *J. Phys. Chem. B* (2014), *118*, 12371-12382.

38. Barbara Chiavarino, Maria Elisa Crestoni, Markus Schütz, Aude Bouchet, Susanna Piccirillo, Vincent Steinmetz, Otto Dopfer, Simonetta Fornarini

 **Cation- interactions in protonated phenylalkylamines**

 *J. Phys. Chem. A* **2014**, *118*, 7130-7138.

37. Bodo, Enrico; Ciavardini, Alessandra; Dalla Cort, Antonella; Giannicchi, Ilaria; Yafteh Mihan, Francesco; Fornarini, Simonetta; Vasile, Silvana; Scuderi, Debora; Piccirillo, Susanna

 **Anion recognition by uranyl-salophen derivatives as probed by infrared multiple photon dissociation spectroscopy spectroscopy and ab-initio modeling**

 *Chem. Eur. J.* (2014), 20, 11783-11792.

36. Francesco Lanucara, Simonetta Fornarini, Claire E. Eyers, Maria Elisa Crestoni

**Probing the exposure of the phosphate group in modified amino acids and peptides by ion-molecule reactions with triethoxyborane in FT-ICR mass spectrometry**

*Rapid Commun. Mass Spectrom.* (2014), 28, 1107–1116

35. Francesco Lanucara, Barbara Chiavarino, Debora Scuderi, Philippe Maitre, Simonetta Fornarini*,* Maria Elisa Crestoni

**Kinetic control in the CID-induced elimination of H3PO4 from phosphorylated serine probed by IRMPD spectroscopy**

*Chem. Commun*. (2014), *50*, 3845-3848.

34. Maria Elisa Crestoni, Francesco Lanucara, Barbara Chiavarino, Simonetta Fornarini

**N-nitrosation of N-acetyltryptophan probed by IR spectroscopy of the gaseous anion**

*Chem. Phys. Lett.* (2013), 588, 215-219

33. Barbara Chiavarino, Maria Elisa Crestoni, Philippe Maitre, Simonetta Fornarini

**Halide adducts of 1,3,5-trinitrobenzene: vibrational signatures and role of anion- interactions**

 *Int. J. Mass Spectrom.* (2013), 354-355, 62-69.

32. Alessandra Ciavardini, Flaminia Rondino, Alessandra Paladini, Maurizio Speranza, Simonetta Fornarini, Mauro Satta, Susanna Piccirillo

**The effect of fluorine substitution in chiral recognition: interplay of CH⋯π, OH⋯π and CH⋯F interactions in gas-phase complexes of 1-aryl-1-ethanol with butan-2-ol.**

*Physical Chemistry Chemical Physics* (2013), 15, 19360-19370.

31. Alberto De Petris, Alessandra Ciavardini, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

**Vibrational Signatures of the Naked Aqua Complexes from Platinum(II) Anticancer Drugs**

*Journal of Physical Chemistry Letters* (2013), 4, 3631-3635.

30. Barbara Chiavarino, Philippe Maitre, Simonetta Fornarini, Maria Elisa Crestoni

**Cyanide-Arene Meisenheimer Complex Generated in Electrospray Ionization Mass Spectrometry Using Acetonitrile as a Solvent**

*J. Am. Soc. Mass Spectrom.* (2013), 24, 1603-1607.

29. Barbara Chiavarino, Maria Elisa Crestoni, Joel Lemaire, Philippe Maitre, Simonetta Fornarini

**Infrared Spectroscopy of Protonated Allyl-trimethylsilane: Evidence for the β-Silyl Effect**

 *J. Chem. Phys.* (2013)**139**, (pp. 071102/1-071102/4)

28. Lanucara, Francesco; Scuderi, Debora; Chiavarino, Barbara; Fornarini, Simonetta; Maitre, Philippe; Crestoni, Maria Elisa

**IR Signature of NO Binding to a Ferrous Heme Center**

*Journal of Physical Chemistry Letters* (2013), 4, 2414-2417.

27. Francesco Lanucara, Maria Elisa Crestoni, Barbara Chiavarino, Simonetta Fornarini, Oscar Hernandez, Debora Scuderi, Philippe Maitre

**Infrared Spectroscopy of Nucleotides in the Gas Phase 2.The Protonated Cyclic 3’,5’-Adenosine Monophosphate**

 *RSC Adv*.(2013), 3, 12711 – 12720.

26. Maria Elisa Crestoni, Barbara Chiavarino,Stefano Guglielmo, Valentina Lilla, Simonetta Fornarini

 **Tandem mass spectrometry of nitric oxide and hydrogen sulfide releasing aspirins: a hint into activity behavior**

*Mass Spectrometry* (2013), 2, A0017/1-A0017/4.

25. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Debora Scuderi, Jean-Yves Salpin

 **Interaction of cisplatin with adenine and guanine: a combined IRMPD, MS/MS and theoretical study**

*J. Am. Chem. Soc.* (2013), 135, 1445-1455.

24. Hans-Ullrich Siehl, Sandra Brixner, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Alberto De Petris, Simonetta Fornarini

 **Isomeric C5H11Si+ ions from the trimethylsilylation of acetylene: an experimental and theoretical study**

*Int. J.Mass Spectrom.* (2013) 334, 58-66.

23. Francesco Lanucara, Barbara Chiavarino, Maria Elisa Crestoni, Debora Scuderi, Rajeev K. Sinha, Philippe Maître, Simonetta Fornarini

 **S-Nitrosation of Cysteine as Evidenced by IRMPD Spectroscopy**

*Int. J.Mass Spectrom.* (2012) 330-332, 160-167.

22. Maria Elisa Crestoni, Barbara Chiavarino, Vincent Steinmetz, Simonetta Fornarini

**Vibrational study of a benzyl carbanion: deprotonated 2,4-dinitrotoluene**
*J. Chem. Phys.* (2012)**137**, 181101 (pp. 181101/1-181101/4).

21. Maria Elisa Crestoni, Barbara Chiavarino, Debora Scuderi, Annito Di Marzio, Simonetta Fornarini

**Discrimination of 4-Hydroxyproline Diastereomers by Vibrational Spectroscopy of the Gaseous Protonated Species**

*Journal of Physical Chemistry B* (2012), 116, 8771-8779.

20. Maria Elisa Crestoni, Simonetta Fornarini

**Jahn-Teller Distortion of Hydrocarbon Cations Probed by IRPD Spectroscopy**

*Angew. Chem. Int. Ed.* (2012), 51, 7373-7375

19. Barbara Chiavarino, Maria Elisa Crestoni, S. Fornarini, S. Taioli, I. Mancini, P. Tosi

**Infrared spectroscopy of copper-resveratrol complexes: a joint experimental and**

**theoretical study**

*J. Chem. Phys.* (2012), **137,** 024307 (pp. 024307/1-024307/9).

18. Barbara Chiavarino, Maria Elisa Crestoni, Otto Dopfer, Philippe Maitre, Simonetta Fornarini

**Benzylium versus Tropylium Ion Dichotomy: Vibrational Spectroscopy of Gaseous C8H9+ Ions**

*Angew. Chem. Int. Ed.* (2012), 51, 4947-4949.

17. **Maria Elisa Crestoni,** [Barbara Chiavarino](http://www.sciencedirect.com/science?_ob=RedirectURL&_method=outwardLink&_partnerName=27983&_origin=article&_zone=art_page&_linkType=scopusAuthorDocuments&_targetURL=http%3A%2F%2Fwww.scopus.com%2Fscopus%2Finward%2Fauthor.url%3FpartnerID%3D10%26rel%3D3.0.0%26sortField%3Dcited%26sortOrder%3Dasc%26author%3DChiavarino,%2520Barbara%26authorID%3D6602709393%26md5%3D3069c793cb9ec78ca7a84ac3c61e8529&_acct=C000058858&_version=1&_userid=2814622&md5=ab6bfa581dd371603d0102bc5019423d)**, Joel Lemaire, Philippe Maitre, Simonetta Fornarini**

**IR spectroscopy of gaseous fluorocarbon ions: the perfluoroethyl anion**

*Chem. Phys.* (2012), 398, 118-123.

16. Rajeev K. Sinha, Barbara Chiavarino, Maria Elisa Crestoni, Debora Scuderi, Simonetta Fornarini

**Tyrosine nitration as evidenced by IRMPD spectroscopy**

*Int. J.Mass Spectrom.* (2011) 308, 209-216.

15. Lin, Yawei; Crestoni, Maria Elisa; Fornarini, Simonetta; Mayer, Paul M.

**A neutralization-reionization and reactivity mass spectrometry study of the generation of neutral hydroxymethylene.**

*J. Mass Spectrom.* (2011), 46, 546-552.

14. Lanucara, Francesco; Chiavarino, Barbara; Crestoni, Maria Elisa; Scuderi, Debora; Sinha, Rajeev K.; Maitre, Philippe; Fornarini, Simonetta.

**Naked Five-Coordinate FeIII(NO) Porphyrin Complexes: Vibrational and Reactivity Features**

*Inorg. Chem.* (2011), 50, 4445-4452.

13. Cecilia Coletti,Nazzareno Re,Debora Scuderi,Philippe Maître,Barbara Chiavarino,

 Simonetta Fornarini,Francesco Lanucara,Rajeev K. Sinha, Maria Elisa Crestoni,

 **IRMPD spectroscopy of gaseous protonated S-nitrosocaptopril, a biologically active, synthetic amino acid**

 *Phys. Chem. Chem. Phys.*, (2010), 12, 13455-13467.

12. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Francesco Lanucara

 **Probing Bare High-Valent Transition Metal−Oxo Complexes: an ESI FT-ICR Study of Reactive Intermediates**

 *European Journal of Mass Spectrometry* (2010),16, 407-414.

11. Sinha, Rajeev K.; Chiavarino, Barbara; Fornarini, Simonetta; Lemaire, Joel; Maitre, Philippe; Crestoni, Maria Elisa.

 **Protonated Sulfuric Acid: Vibrational Signatures of the Naked Ion in the Near- and Mid-IR**

 *Journal of Physical Chemistry Letters* (2010), 1, 1721-1724.

10. Rajeev K. Sinha, Philippe Maître, Susanna Piccirillo, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini

 **Cysteine radical cation: a distonic structure probed by gas phase IR spectroscopy**

 *Phys. Chem. Chem. Phys.* (2010), 12, 9794 – 9800.

9. Crestoni, Maria Elisa; Fornarini, Simonetta; Lanucara, Francesco; Warren, Jeffrey J.; Mayer, James M.

 **Probing Spin-Forbidden' Oxygen-Atom Transfer: Gas-Phase Reactions of Chromium-Porphyrin Complexes**

 *Journal of the American Chemical Society* (2010), 132, 4336-4343.

8. Maria Elisa Crestoni, Simonetta Fornarini, Francesco Lanucara

 **Oxygen-Atom Transfer by a Naked Manganese(V)–Oxo–Porphyrin Complex Reveals Axial Ligand Effect**

 *Chem. Eur. J*. (2009), 15, 7863-7866.

7. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Francesco Lanucara, Joel Lemaire, Philippe Maitre, Debora Scuderi

 **Molecular complexes of simple anions with electron-deficient arenes: spectroscopic evidence for two types of structural motifs for anion-arene interactions**

 *Chem. Eur. J*. (2009), 15, 8185-8195.

6. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Francesco Lanucara, Joel Lemaire, Philippe Maitre

 **Mid-IR Spectroscopy and Structural Features of Protonated Carbonic Acid in the Gas Phase**

 *ChemPhysChem* (2009) 10, 520-522.

5. B. Chiavarino,M. E. Crestoni, B. Di Rienzo, S. Fornarini, F. Lanucara

 **Site-selectivity of Protonation in Gaseous Toluene**

 *Phys. Chem. Chem. Phys.* (2008), 10, 5507-5509.

4. B. Chiavarino,M. E. Crestoni, S. Fornarini, C. Rovira

 **Unravelling the Intrinsic Features of NO Binding to Iron(II)- and Iron(III)-hemes**

 *Inorg. Chem.* (2008) 47, 7792-7801.

3. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Francesco Lanucara, Joel Lemaire, Philippe Maitre, and Debora Scuderi

 **Direct Probe of NO Vibration in the Naked Ferric Heme Nitrosyl Complex**

 *ChemPhysChem* (2008) 9, 826-828

2. Barbara Chiavarino, Romano Cipollini, Maria Elisa Crestoni, Simonetta Fornarini,\* Francesco Lanucara, Andrea Lapi

 **Probing the Compound I-like Reactivity of a Bare High-Valent Oxo Iron Porphyrin Complex: the Oxidation of Tertiary Amines**

 *J. Am. Chem. Soc.* (2008) 130, 3208-3217.

1. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Francesco Lanucara, Joel Lemaire, Philippe Maitre, and Debora Scuderi

 **Infrared Spectroscopy of Isolated Nucleotides. 1. The cyclic 3’,5’-Adenosine Monophosphate Anion**

 *Int. J. Mass Spectrom.* (2008), 270, 111-117.