FORMATO EUROPEO PER IL CURRICULUM VITAE

INFORMAZIONI PERSONALI

Nome	**FORNARINI SIMONETTA**
Nazionalità	italiana

ESPERIENZA LAVORATIVA

• da 12/03/2024 ad oggi	Professore emerito (D.M. 12.03.2024 n. 509)
• da 1/11/2022 ad oggi	Professore in quiescenza - Docente EAQ presso il Dipartimento di Chimica e Tecnologie del Farmaco – facoltà di Farmacia e Medicina – Sapienza Università di Roma
• 2000-2022	Professore ordinario di Chimica Generale e Inorganica (CHIM/03) – facoltà di Farmacia e Medicina – Sapienza Università di Roma
• 1992-2000	Professore associato di Chimica Generale e Inorganica (CHIM/03) – facoltà di Farmacia – Sapienza Università di Roma
• 1983-1992	Ricercatore universitario (CHIM/03) – facoltà di Farmacia – Sapienza Università di Roma
• 1981-1983	Ricercatore CNR – Istituto di Chimica nucleare – Area della ricerca di Montelibretti

ISTRUZIONE E FORMAZIONE

• 1978-1979	Research assistantship – University of California Santa Cruz
• 1971-1976	Corso di laurea in Chimica – Università degli Studi di Roma La Sapienza
• 1966-1971	Liceo classico T. Tasso in Roma

CAPACITÀ E COMPETENZE PERSONALI

Acquisite nel corso della vita e della carriera ma non necessariamente riconosciute da certificati e diplomi ufficiali.

MADRELINGUA	**ITALIANO**
ALTRE LINGUA	
	INGLESE
• Capacità di lettura	[eccellente]
• Capacità di scrittura	[eccellente]
• Capacità di espressione orale	[eccellente]

CAPACITÀ E COMPETENZE RELAZIONALI

Vivere e lavorare con altre persone, in ambiente multiculturale, occupando posti in cui la comunicazione è importante e in situazioni in cui è essenziale lavorare in

Ha trascorso periodi di ricerca presso università in USA sia da neolaureata, sia come visiting professor tramite scholarship della fondazione Fulbright.
Ha presentato numerose relazioni su invito a conferenze internazionali (e. g. ESOR, ESOC, KISPOC, IMSC, IUPAC) e presso università italiane e straniere (in USA, Canada, Europa).

squadra (ad es. cultura e sport), ecc.

CAPACITÀ E COMPETENZE ORGANIZZATIVE

Ad es. coordinamento e amministrazione di persone, progetti, bilanci; sul posto di lavoro, in attività di volontariato (ad es. cultura e sport), a casa, ecc.

I suoi incarichi istituzionali presso l'Ateneo includono la presidenza del Consiglio di corso di studi in CTF con una prima elezione nel 2001 e successivamente per altri due mandati a partire dal 2007.
A livello nazionale ha svolto il ruolo di Presidente della Commissione per l'Abilitazione Scientifica Nazionale 2021-2023 alla prima e seconda fascia dei professori universitari nel settore concorsuale 03/B1- Fondamenti delle Scienze Chimiche e Sistemi Inorganici

CAPACITÀ E COMPETENZE TECNICHE

Con computer, attrezzature specifiche, macchinari, ecc.

I suoi interessi di ricerca si sono rivolti allo studio di aspetti fondamentali di reazioni chimiche, rilevanti in particolare in ambito bio-inorganico, caratterizzandone meccanismi, intermedi elusivi, struttura di reagenti e prodotti ed operando prevalentemente su molecole o cluster molecolari prelevati dalla soluzione ed isolati in fase gassosa. Le sue pubblicazioni (circa 190) includono capitoli di libri e rassegne pubblicate su riviste autorevoli quali Chemical Reviews e Accounts of Chemical Research. Globalmente risultano corrispondere ad un HI di 35 ed un impact factor totale superiore a 1000. Nell'ambito della comunità scientifica nazionale ha per prima individuato il potenziale della spettroscopia multifotonica IR accoppiata alla spettrometria di massa per rivelare la struttura di intermedi ionici elusivi (e. g. benzene protonato Angew. Chem. Int. Ed. 2003) risolvendo problematiche oggetto di ampia discussione e risonanza.

CAPACITÀ E COMPETENZE ARTISTICHE

Musica, scrittura, disegno ecc.

[Descrivere tali competenze e indicare dove sono state acquisite.]

ALTRE CAPACITÀ E COMPETENZE

Competenze non precedentemente indicate.

PATENTE O PATENTI

ULTERIORI INFORMAZIONI

[Inserire qui ogni altra informazione pertinente, ad esempio persone di riferimento, referenze ecc.]

ALLEGATI

ELENCO PUBBLICAZIONI

194. **Protonated Forms of Naringenin and Naringenin Chalcone: Proteiform Bioactive Species Elucidated by IRMPD Spectroscopy, IMS, CID-MS, and Computational Approaches**
Davide Corinti, Lucretia Rotari, Maria Elisa Crestoni, Simonetta Fornarini, Jos Oomens, Giel Berden, Aura Tintaru, and Barbara Chiavarino*
J. Agric. Food Chem. 2023, 71, 4005-4015

193. **IRMPD spectroscopy and quantum-chemical simulations of the reaction products of cisplatin with the dipeptide CysGly**
Davide Corinti *,Roberto Paciotti *, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Gilles Frison, Maria Elisa Crestoni, Simonetta Fornarini
J. Inorganic Biochemistry 247 (2023) 112342

192. **Binding Motifs of Carboplatin and Oxaliplatin with Guanine: A Combined MS/MS, IRMPD, and Theoretical Study**
Barbara Chiavarino,* Lucretia Rotari, Maria Elisa Crestoni, Davide Corinti, Simonetta Fornarini, Debora Scuderi, Jean-Yves Salpin* Inorg. Chem. 2023, 62, 14546-14558

191. **Binding Modes of a Cytotoxic Dinuclear Copper(II) Complex with Phosphate Ligands Probed by Vibrational Photodissociation Ion Spectroscopy**
Marco Giampà, Davide Corinti,* Alessandro Maccelli, Simonetta Fornarini, Giel Berden, Jos Oomens, Sabrina Schwarzbich, Thorsten Glaser, Maria Elisa Crestoni*
Inorg. Chem. 2023, 62, 1341−1353 https://doi.org/10.1021/acs.inorgchem.2c02091

190. **Elusive intermediates in cisplatin reaction with target amino acids: Platinum(II)-cysteine complexes assayed by IR ion spectroscopy and DFT calculations**
Davide Corinti,* Roberto Paciotti,* Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini
J. Inorganic Biochemistry 2022, 237, 112017 (1-11) https://doi.org/10.1016/j.jinorgbio.2022.112017

189. **Ligation motifs in zinc bound sulfonamide drugs assayed by IR ion spectroscopy**
Davide Corinti,* Barbara Chiavarino, Philippe Maitre, Maria Elisa Crestoni, Simonetta Fornarini*
Molecules 2022, 27, 3144 (1-13) doi: 10.3390/molecules27103144

188. **IRMPD spectroscopy of bare monodeprotonated genistein, an antioxidant flavonoid**
R. Paciotti, B. Chiavarino, C. Coletti,* D. Scuderi, N. Re, D. Corinti, L. Rotari, S. Fornarini, M. E. Crestoni*
ACS Omega **2022**, 7, 19535−19544 doi: 10.1021/acsomega.2c01236

187. **Cation-π interactions between a noble metal and a polyfunctional aromatic ligand: Ag+(benzylamine)**
Davide Corinti, Alessandro Maccelli, Barbara Chiavarino, Markus Schütz, Aude Bouchet, Otto Dopfer,* Maria Elisa Crestoni, Simonetta Fornarini*
Chem. Eur. J. 2022, 28, e202200300 (1-11) https://doi.org/10.1002/chem.202200300

186. **Prevailing Charge Transfer in the Reaction of Protonated and Neutral Nitric Oxide: A Theoretical and Experimental Study**
Usharani,* Dandamudi; Crestoni, Maria Elisa; Fornarini,* Simonetta Int. J. Mass Spectrom. **2022**, 471, 116724.

185. **Molecular basis for the remarkably different gas-phase behavior of deprotonated thyroid hormones triiodothyronine (T3) and reverse triiodothyronine (rT3): a clue for their discrimination?**
Davide Corinti*, Barbara Chiavarino, Mattia Spano, Aura Tintaru, Simonetta Fornarini, Maria Elisa Crestoni*
Anal. Chem. **2021**, 93, 14869-14877. https://pubs.acs.org/doi/abs/10.1021/acs.analchem.1c03892

184. **Metabolomic profiling of fresh Goji (Lycium barbarum L.) berries from two cultivars grown in Center Italy: a multi-methodological approach**
Mattia Spano, Alessandro Maccelli, Giacomo Di Matteo, Cinzia Ingallina, Mariangela Biava, Maria Elisa Crestoni,*, Jean-Xavier Bardaud, Anna Maria Giusti, Anna Scotto D'Abusco, Anatoly P. Sobolev,* Alba Lasalvia, Simonetta Fornarini, Luisa Mannina Molecules **2021**, *26*, 5412 (1-23) 10.3390/molecules26175412

183. **From preassociation to chelation: a survey of cisplatin interaction with methionine at molecular level by IR ion spectroscopy and computations**
Roberto Paciotti, Davide Corinti, Philippe Maitre, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini* J. Am. Soc. Mass Spectrom. **2021**, 32, 2206−2217
https://doi.org/10.1021/jasms.1c00152

182. **Molecular properties of bare and microhydrated vitamin B5 - calcium complexes**
Davide Corinti, Barbara Chiavarino, Debora Scuderi, Philippe Maitre, Caterina Fraschetti, Antonello Filippi, Simonetta Fornarini, Maria Elisa Crestoni* Int. J. Molecular Sciences **2021**, 22, 692 (pp. 1-19)

181. **Binding motifs in the naked complexes of target amino acids with an excerpt of antitumor active biomolecule. An ion vibrational spectroscopy assay**
Barbara Chiavarino, Rajeev K. Sinha, Maria Elisa Crestoni, Davide Corinti, Antonello Filippi, Caterina Fraschetti, Debora Scuderi, Philippe Maitre, Simonetta Fornarini* Chem. Eur. J. **2021**, 27, 2348-2360.
DOI: 10.1002/chem.202003555

180. **Chemico-biological characterization of Torpedino di Fondi® tomato fruits: a comparison with San Marzano cultivar at two ripeness stages**
Cinzia Ingallina, Alessandro Maccelli, Mattia Spano, Giacomo Di Matteo, Antonella Di Sotto, Anna Maria Giusti, Giuliana Vinci, Silvia Di Giacomo, Mattia Rapa, Salvatore Ciano, Caterina Fraschetti, Antonello Filippi, Giovanna Simonetti, Carlos Cordeiro, Marta Sousa Silva, Maria Elisa Crestoni *, Anatoly P. Sobolev*, Simonetta Fornarini, Luisa Mannina
Antioxidants **2020**, 9, 1027 (1-29).

179. **Can an elusive Pt(III) oxidation state be exposed in an isolated complex?**
Corinti,* Davide; Frison, Gilles; Chiavarino, Barbara; Gabano, Elisabetta; Osella, Domenico; Crestoni, Maria Elisa; Fornarini,* Simonetta
Angew. Chem. Int. Ed. **2020**, 59, 15595-15598; *Angew. Chemie* **2020**, *132*, 15725-15728.

178. **Metabolic profiling of different wild and cultivated Allium species based on high resolution mass spectrometry, HPLC-PDA and color analysis**
Alessandro Maccelli, Stefania Cesa, Francesco Cairone, Daniela Secci, Luigi Menghini, Barbara Chiavarino, Simonetta Fornarini, Maria Elisa Crestoni*, Marcello Locatelli
J. Mass Spectrom. **2020**, 55, 2020e4525. doi.org/10.1002/jms.4525

177. **A multi-methodological inquiry of the behavior of cisplatin-based Pt(IV) derivatives in the presence of bioreductants with a focus on the isolated encounter complexes**
Corinti,* Davide; Crestoni, Maria Elisa; Fornarini, Simonetta; Dabbish,* Eslam ; Sicilia, Emilia; Gabano,* Elisabetta; Perin, Elena; Osella, Domenico J. Biol. Inorg. Chem. **2020**, 25, 655-670.
https://rdcu.be/b3BdV DOI:10.1007/s00775-020-01789-w

176. **Insights into Cisplatin Binding to Uracil and Thiouracils from IRMPD Spectroscopy and Tandem Mass Spectrometry**
Corinti, Davide; Crestoni,* Maria Elisa; Chiavarino, Barbara; Fornarini, Simonetta; Scuderi, Debora; Salpin,* Jean-Yves J. Am. Soc. Mass Spectrom. **2020**, 31, 946-960. DOI: 10.1021/jasms.0c00006

175. **IRMPD spectra of protonated hydroxybenzaldehydes: Evidence of torsional barriers in carboxonium ions**
Barbara Chiavarino*, Otto Dopfer, Maria Elisa Crestoni, Davide Corinti, Philippe Maître, Simonetta Fornarini ChemPhysChem **2020**, 21, 749-761. DOI: 10.1002/cphc.202000041

174. Maitre,* Philippe; Scuderi, Debora; Corinti, Davide; Chiavarino, Barbara; Crestoni, Maria Elisa; Fornarini,* Simonetta
Applications of IRMPD to the detection of post translational modifications
Chem. Rev. **2020**, 120, 3261-3295. https://doi.org/10.1021/acs.chemrev.9b00395

173. Alessandro Maccelli, Luca Vitanza, Anna Imbriano, Caterina Fraschetti, Antonello Filippi, Paola Goldoni, Linda Maurizi, Maria Grazia Ammendolia, Maria Elisa Crestoni, Simonetta Fornarini, Luigi Menghini, Carlotta Marianecci, Maria Carafa, Catia Longhi *, Federica Rinaldi
***Satureja montana* L. essential oils: chemical profiles/phytochemical screening, antimicrobial activity and O/W NanoEmulsion formulations**
Pharmaceutics **2020**, 12, 7 pp. 1-20 doi: 10.3390/pharmaceutics12010007

172. Cinzia Ingallina; Donatella Capitani; Simone Carradori; Marcello Locatelli; Antonella Di Sotto; Silvia Di Giacomo; Chiara Toniolo; Gabriella Pasqua; Alessio Valletta; Giovanna Simonetti; Alessia Parroni; Marzia Beccaccioli; Giuliana Vinci; Mattia Rapa; Anna Maria Giusti; Caterina Fraschetti; Antonello Filippi; Alessandro Maccelli; Maria Elisa Crestoni; Simonetta Fornarini; Anatoly P Sobolev; Luisa Mannina*
Phytochemical and biological characterization of Italian "sedano bianco di Sperlonga" Protected Geographical Indication celery ecotype: a multimethodological approach
Food Chemistry **2020**, 309, article 125649, pp. 1-15

171. Davide Corinti, Roberto Paciotti, Nazzareno Re, Cecilia Coletti, Barbara Chiavarino, Maria Elisa Crestoni and Simonetta Fornarini*
Binding motifs of cisplatin interaction with simple biomolecules and aminoacid targets probed by IR ion spectroscopy
Pure Appl. Chem. **2020**, 92, 3–13. DOI: https://doi.org/10.1515/pac-2019-0110

170. Davide Corinti*, Alessandro Maccelli, Maria Elisa Crestoni, Stefania Cesa, Deborah Quaglio, Bruno Botta, Cinzia Ingallina,Luisa Mannina, Aura Tintaru, Barbara Chiavarino*, Simonetta Fornarini*
IR ion spectroscopy in a combined approach with MS/MS and IM-MS to discriminate epimeric anthocyanin glycosides (cyanidin 3-O-glucoside and -galactoside)
Int. J. Mass Spectrom. **2019**, 444, article 116179 DOI: 10.1016/j.ijms.2019.116179

169. D. Corinti, M. E. Crestoni, S. Fornarini*,F. Ponte, N. Russo, E. Sicilia*, E. Gabano, D. Osella*
Elusive intermediates in the breakdown reactivity patterns of prodrug platinum(IV) complexes
J. Am. Soc. Mass Spectrom. **2019**, 30, 1881-1894 DOI: 10.1007/s13361-019-02186-7

168. Macaluso, Veronica; Scuderi, Debora; Crestoni, Maria Elisa; Fornarini, Simonetta; Corinti, Davide; Dalloz, Enzo; Martínez-Núñez, Emilio; Hase, William; Spezia*, Riccardo
L-Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations
J. Phys. Chem. A **2019**, 123, 3685-3696. DOI: 10.1021/acs.jpca.9b01779

167. Davide Corinti, Alessandro Maccelli, Barbara Chiavarino, Philippe Maitre, Debora Scuderi, Enrico Bodo, Simonetta Fornarini, and Maria Elisa Crestoni*
Vibrational Signatures of Curcumin's Chelation in copper(II) complexes: an appraisal by IRMPD spectroscopy
J. Chem. Phys. **150**, 165101/1-12 (**2019**); https://doi.org/10.1063/1.5086666

166. Ciavardini, Alessandra; Coreno, Marcello; Callegari, Carlo; Spezzani, Carlo; De Ninno, Giovanni; Ressel, Barbara; Grazioli, Cesare; de Simone, Monica; Kivimäki, Antti; Miotti, Paolo; Frassetto, Fabio; Poletto, Luca; Puglia, Carla; Fornarini, Simonetta; Bodo, Enrico; Piccirillo, Susanna
Ultra-fast -VUV photoemission study of UV excited 2-nitrophenol
J. Phys. Chem. A, **2019**, *123*, 1295–1302. DOI: 10.1021/acs.jpca.8b10136

165. Davide Corinti, Maria Elisa Crestoni, Simonetta Fornarini*, Maren Pieper, Karsten Niehaus, Marco Giampà*
An integrated approach to study novel properties of a MALDI matrix (4-maleicanhydridoproton sponge) for MS imaging analyses
Analytical and Bioanalytical Chemistry (**2019**) 411:953–964 https://doi.org/10.1007/s00216-018-1531-7

164. Davide Corinti, Cecilia Coletti, Nazzareno Re, Roberto Paciotti, Philippe Maitre, Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini*
Short-lived intermediates (encounter complexes) in cisplatin ligand exchange elucidated by infrared ion spectroscopy
Int. J.Mass Spectrom. **2019**, 435, 7–17. https://doi.org/10.1016/j.ijms.2018.10.012

163. Luca Vitanza, Alessandro Maccelli, Massimiliano Marazzato, Francesca Scazzocchio, Antonella Comanducci, Simonetta Fornarini, Maria Elisa Crestoni, Antonello Filippi, Caterina Fraschetti, Federica Rinaldi, Marta Aleandri, Paola Goldoni, Maria Pia Conte, Maria Grazia Ammendolia*, Catia Longhi*
Satureja montana L. essential oil and its antimicrobial activity alone or in combination with gentamicin
Microbial Pathogenesis 126 (**2019**) 323–331

162. 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. http://dx.doi.org/10.1002/ejic.201800273

161. Davide Corinti, Daniele Catone, Stefano Turchini, Flaminia Rondino, Maria Elisa Crestoni, Simonetta Fornarini*
Photoionization mass spectrometry of ω-phenylalkylamines: role of radical cation-π interaction
J. Chem. Phys. **2018**, 148, 164307/1-8. https://doi.org/10.1063/1.5027786 DOI: 10.1063/1.5027786

160. 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. doi.org/10.1016/j.foodchem.2018.02.050

159. 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.

158. 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 and Simonetta Fornarini
Cisplatin and transplatin interaction with methionine: bonding motifs assayed by vibrational spectroscopy in the isolated ionic complexes
Physical Chemistry Chemical Physics, **2017**, 19, 26697-26707.

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

156. Barbara Chiavarino, Maria Elisa Crestoni, Simonetta Fornarini, Debora Scuderi and 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

155. 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.

154. 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
Journal of Molecular Spectroscopy 335 (**2017**) 108–116.

153. 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.

152. 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.

151. 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.

150. 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

149. 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.

148. 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

147. 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.

146. 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. **2015**, *17*, 25891-25904.

145. 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 NH_3^+-π interaction
Phys. Chem. Chem. Phys. **2015**, *17*, 25742-25754.

144. 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*, pp 1605–1610

143. Maria Elisa Crestoni, Barbara Chiavarino, Simonetta Fornarini
Nitrosyl-Heme and Anion-Arene Complexes: Structure, Reactivity and Spectroscopy
Pure and Applied Chemistry **2015**, 87(4), 379-390.

142. 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.

141. 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.

140. 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.

139. 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
Chemical Science (Chem. Sci.), **2015**, *6*, 1516 – 1529.

138. 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.

137. 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.

136. 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.

135. 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.

134. 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

133. Francesco Lanucara, Barbara Chiavarino, Debora Scuderi, Philippe Maitre, Simonetta Fornarini, Maria Elisa Crestoni
Kinetic control in the CID-induced elimination of H_3PO_4 from phosphorylated serine probed by IRMPD spectroscopy
Chem. Commun., **2014**, *50*, 3845-3848.

132. 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

131. 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.

130. 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(44), 19360-19370.

129. 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(21), 3631-3635.

128. 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 (no.10), 1603-1607.

127. Barbara Chiavarino, Maria Elisa Crestoni, Joel Lemaire, Philippe Maitre, and Simonetta Fornarini
Infrared Spectroscopy of Protonated Allyl-trimethylsilane: Evidence for the β-Silyl Effect
J. Chem. Phys. **139**, (pp. 071102/1-071102/4) (**2013**)

126. 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(15), 2414-2417.

125. 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 (31), 12711 – 12720.

124. 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.

123. 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.

122. Hans-Ullrich Siehl, Sandra Brixner, Cecilia Coletti, Nazzareno Re, Barbara Chiavarino, Maria Elisa Crestoni, Alberto De Petris, Simonetta Fornarini
Isomeric $C_5H_{11}Si^+$ ions from the trimethylsilylation of acetylene: an experimental and theoretical study
Int. J.Mass Spectrom. 334 (**2013**), pp. 58-66.

121. 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. 330-332 (2012), 160-167.

120. Maria Elisa Crestoni, Barbara Chiavarino, Vincent Steinmetz, and Simonetta Fornarini
Vibrational study of a benzyl carbanion: deprotonated 2,4-dinitrotoluene
J. Chem. Phys. **137**, 181101 (pp. 181101/1-181101/4) (2012)

119. 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

118. Maria Elisa Crestoni, Simonetta Fornarini
Jahn-Teller Distortion of Hydrocarbon Cations Probed by IRPD Spectroscopy

Angew. Chem. Int. Ed. 2012, 51, 7373-7375

117. 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) (2012)

116. Barbara Chiavarino, Maria Elisa Crestoni, Otto Dopfer, Philippe Maitre, Simonetta Fornarini
Benzylium versus Tropylium Ion Dichotomy: Vibrational Spectroscopy of Gaseous $C_8H_9^+$ Ions
Angew. Chem. Int. Ed. 2012, 51, 4947-4949.

115. Maria Elisa Crestoni, Barbara Chiavarino, Joel Lemaire, Philippe Maitre, Simonetta Fornarini
IR spectroscopy of gaseous fluorocarbon ions: the perfluoroethyl anion
Chem Phys 2012, 398, 118-123.

114. Rajeev K. Sinha, Barbara Chiavarino, Maria Elisa Crestoni, Debora Scuderi, Simonetta Fornarini
Tyrosine nitration as evidenced by IRMPD spectroscopy
Int. J.Mass Spectrom. 308 (2011), pp. 209-216

113. 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.

112. 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

111. 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

110. 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.

109. 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(11), 1721-1724.

108. 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

107. 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(12), 4336-4343.

106. 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.

105. 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

104. 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 **10**, 520-522 (2009)

103. 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

102. 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. **47** (17), 7792-7801 (2008)

101. 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 **9**, 826-828 (2008)

100. 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.

99. 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.

98. M. E. Crestoni, S. Fornarini
"Compound I of Naked Heme (Iron-Protoporphyrin IX)"
Inorg. Chem. **46** (22), 9018-9020 (2007)

97. U. J. Lorenz, J. Lemaire, P. Maitre, M. E. Crestoni, S. Fornarini, O. Dopfer
"Protonation of Heterocyclic Aromatic Molecules: IR Signature of the Protonation Site of Furan and Pyrrole"
Int. J. Mass Spectrom. (2007), **267**, 43-53.

96. B. Chiavarino, M. E. Crestoni, S. Fornarini, F. Lanucara, J. Lemaire, P. Maître
"Meisenheimer Complexes Positively Characterized as Stable Intermediates in the Gas Phase"
Angew. Chem. Int. Ed. **46**, 1995-1998 (2007).

95. B. Chiavarino, M. E. Crestoni, S. Fornarini, C. Rovira
"Protonated Heme"
Chem. Eur. J. **13**, 776-785 (2007).

94. M. E. Crestoni, S. Fornarini
"Heme-peptide/protein ions and phosphorous ligands: search for site-specific addition reactions"
J. Biol. Inorg. Chem. (2007), 12(1), 22-35.

93. B. Chiavarino, M. E. Crestoni, S. Fornarini, J. Lemaire, P. Maître, L. McAleese
"π-Complex Structure of Gaseous Benzene-NO Cations Assayed by IR Multiple Photon Dissociation Spectroscopy"
J. Am. Chem. Soc. (2006) **128**, 12553-12561

92. B. Chiavarino, M. E. Crestoni, S. Fornarini, O. Dopfer, J. Lemaire, P. Maître
"IR spectroscopic features of gaseous $C_7H_7O^+$ ions: benzylium versus tropylium ion structures"
J. Phys. Chem. A (2006), **110**(30), 9352-9360

91. O. Dopfer, J. Lemaire, P. Maitre, B. Chiavarino, M. E. Crestoni, S. Fornarini
"IR Spectroscopy of Protonated Toluene: Probing Ring Hydrogen Shifts in Gaseous Arenium Ions"
Int. J. Mass Spectrom. (2006), **249-250**, 149-154.

90. O. Dopfer, N. Solcà, J. Lemaire, P. Maitre, M. E. Crestoni, S. Fornarini
"Protonation Sites of Isolated Fluorobenzene Revealed by IR Spectroscopy in the Fingerprint Range"
J. Phys. Chem. A (2005), 109(20), 7881-7887.

89. G. de Petris, S. Fornarini, M. E. Crestoni, A. Troiani, P. M. Mayer
"What Ion is Generated When Ionizing Acetonitrile?"
J. Phys. Chem. A (2005), 109(20), 4425-4427.

88. M. E. Crestoni, S. Fornarini
"Probing the cytochrome P450-like reactivity of high-valent oxo iron intermediates in the gas phase"
Inorg. Chem. **44** (15), 5379-5387 (2005)

87. F. Angelelli, B. Chiavarino, M. E. Crestoni, S. Fornarini
"Binding of Gaseous Fe(III)-Heme Cation to Model Biological Molecules: Direct Association and Ligand Transfer Reactions."
J. Am. Soc. Mass Spectrom. (2005), 16(4), 589-598.

86. B. Chiavarino, M. E. Crestoni, S. Fornarini, J. Lemaire, L. Mac Aleese, P. Maitre
"Infrared Spectroscopy of Protonated Phenylsilane in the Gas Phase"
ChemPhysChem **6**, 437-440 (2005).

85. S. Fornarini
" Ion structures produced in gas phase radiolysis "

in **Vol. 4.** Fundamentals of and Applications to Organic (and Organometallic) Compounds N. M. M. Nibbering Volume Editor *Encyclopedia of Mass Spectrometry* M. L. Gross, R. M. Caprioli Editors, Vol.4 (2005) chpt. 2, pp. 253-260, Elsevier, Oxford, GB.

84. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Gas phase protonation of benzocycloalkenes"
Eur. J. Mass Spectrom. **10**, 881-887 (2004).

83. B. Chiavarino, M. E. Crestoni, S. Fornarini, J. Lemaire, L. Mac Aleese, P. Maitre
"Infrared Absorption Features of Gaseous Isopropyl Carbocations"
ChemPhysChem **5**, 1679-1685 (2004).

82. M. E. Crestoni, S. Fornarini
" FT-ICR study of the gas phase basicity of N-nitroso-dimethylamine"
J. Mass Spectrom. **39**, 1379-1381 (2004). (IF 2.88 *2004*)

81. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Chemistry of Protonated Species in Gaseous Environments"
plenary lecture at the ESOR 9 conference
J. Phys. Org. Chem. **17**, 957-966 (2004). (IF 1.18 *2004*)

80. B. Chiavarino, M. E. Crestoni, S. Fornarini
" Cation-π Interactions in Gaseous ω-Phenylalkyloxonium Ions "
Int. J. Mass Spectrom. **235**, 145-154 (2004). (IF 2.36 *2004*)

79. M. E. Crestoni, S. Fornarini
" Gas-phase hydrogen/deuterium exchange of adenine nucleotides"
J. Mass Spectrom. **38**, 854-861 (2003). (IF 2.88 *2004*)

78. B. Chiavarino, M. E. Crestoni, S. Fornarini, D. Kuck
" Cation-π Interactions in the Gas Phase Methylation of α,ω-Diphenylalkanes"
J. Phys. Chem. A **107**, 4619-4624 (2003). (IF 2.79 *2004*)

77. W. Jones, P. Boissel, B. Chiavarino, M. E. Crestoni*, S. Fornarini, J. Lemaire, P. Maitre*
" Infrared fingerprint of protonated benzene "
Angew. Chem. Int. Ed. Engl. **42**, 2057-2059 (2003). (IF 8.43 *2004*)
Angew. Chem. **115**, 2103-2105 (2003).

76. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Gas phase regioselectivity in the deprotonation of p-cresol radical cation"
Chem. Phys. Lett. **372**, 183 – 186 (2003). (IF 2.44 *2004*)

75. B. Chiavarino, M. E. Crestoni, S. Fornarini
"The Trimethylsilylation of Acetylene"
Chem. Commun. 1418-1419 (2002). (IF 4.03 *2004*)

74. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Gas Phase Dioxygen Activation by Binuclear Manganese Clusters"
Chem. Eur. J. **8**, 2740-2746 (2002). (IF 4.35 *2004*)

73. E. Baciocchi, M. Bietti, B. Chiavarino, M. E. Crestoni, S. Fornarini
"The Deprotonation of Benzyl Alcohol Radical Cations: a Mechanistic Dichotomy in the Gas Phase as in Solution"

Chem. Eur. J. **8**, 532 (2002).

72. S. Fornarini
"Ion-molecule Reactions of Silicon Cations"
The Chemistry of Organic Silicon Compounds Vol. 3, Eds. Z. Rappoport and Y. Apeloig, Wiley, New York, 2001, pp. 1027-1057.

71. B. Chiavarino, M. E. Crestoni, A. A. Fokin, S. Fornarini
"The Protonation of Gaseous Cyclopropane"
Chem. Eur. J. **7**, 2916-2921 (2001).

70. B. Chiavarino, M. E. Crestoni, S. Fornarini
"A Gas Phase Study of the Ionic Alkylation of Benzocycloalkenes"
J. Am. Chem. Soc. **122**, 5397-5398 (2000). **DOI:** 10.1021/ja000164f

69. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Gas Phase Reactivity of Organosilane Radical Cations. A FT-ICR Study"
Organometallics **19**, 844-848 (2000).

68. B. Chiavarino, M. E. Crestoni, A. Di Marzio, S. Fornarini, M. Rosi
"Gas Phase Ion Chemistry of Borazine, an Inorganic Analogue of Benzene"
J. Am. Chem. Soc. **121**, 11204-11210 (1999). **DOI:** 10.1021/ja992220m

67. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Electrophilic Substitution of Gaseous Borazine"
J. Am. Chem. Soc. **121**, 2619-2620 (1999). **DOI:** 10.1021/ja983799b

66. S. Fornarini, M. E. Crestoni
"Gaseous Arenium Ions at Atmospheric Pressure: Elementary Reactions and Internal Solvation Effects"
Acc. Chem. Res. **31**, 827-834 (1998). **DOI:** 10.1021/ar960247u

65. B. Chiavarino, M. E. Crestoni, B. Di Rienzo, S. Fornarini
"Gas Phase H/D Exchange between Arenium Ions and Selected Bases. The Site of Protonation of Simple Aromatics"
J. Am. Chem. Soc. **120**, 10856-10862 (1998). **DOI:** 10.1021/ja981488v

64. B. Chiavarino, M. E. Crestoni, A. Di Marzio, S. Fornarini
"Determination of Sulfonamide Antibiotics by Gas Chromatography Coupled with Atomic Emission Detection"
J. Chromat. B, Biochem. Sciences Applications **706**, 269-277 (1998).

63. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Radiolytic Silylation of Alkenes and Alkynes by Gaseous Me_3Si^+ Ions. Stereochemical Evidence for the □ Silyl Effect"
J. Am. Chem. Soc. **120**, 1523-1527 (1998). **DOI:** 10.1021/ja9734152

62. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Gas Phase Germylation of Simple Aromatics by Me_3Ge^+ Ions."
J. Organometal. Chem. **545/546**, 53-59 (1997).

61. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Gas Phase Alkylation of Phenyltrimethylgermanes."
J. Organometal. Chem. **545/546**, 45-51 (1997).

60. R. Cipollini, M. E. Crestoni, S. Fornarini
"Positive Ion Chemistry of Elemental Fluorine"
J. Am. Chem. Soc. **119**, 9499 (1997).

59. C. H. DePuy, R. Gareyev, S. Fornarini
"Generation and Assay of $C_6H_xD_{(7-x)}$ (x = 1-6) Benzenium ions. A FA-SIFT Study."
Int. J. Mass Spectrom. Ion Processes **161**, 41-45 (1997).

58. S. Fornarini
"Mechanistic Views on Aromatic Substitution Reactions by Gaseous Cations"
Mass Spectrom. Rev. **15**, 365-389 (1996)

57. M. Aschi, B. Chiavarino, M. E. Crestoni, S. Fornarini
"Structure and Reactivity of Protonated α,α,α-Trifluorotoluene in the Gas Phase. A Combined FT-ICR, Radiolytic and ab Initio MO Study"

J. Phys. Chem. **100**, 19859 (1996) 10.1021/jp961075l

56. B. Chiavarino, M. E. Crestoni, S. Fornarini, C. H. DePuy, R. Gareyev
"Brønsted Acid Behavior of $C_6(H,D)_7^+$ Benzenium Ions A Combined Approach by Radiolytic, FA-SIFT, and FT-ICR Methodologies"

J. Phys. Chem., **100**, 16201-16208 (1996). **DOI:** 10.1021/jp961322l

55. M. E. Crestoni, S. Fornarini
"Reactions of Bare and Ligated Chromium (I) Ions with Gaseous Arenes. Role of a "Spectator" Aromatic Ring in Chelate Complex Formation"

Organometallics **15**, 5695-5700 (1996) DOI: 10.1021/om960459v

54. M. E. Crestoni, S. Fornarini, M. Lentini, M. Speranza
"Hydride Ion Transfer Reaction in the Gas Phase. 2. Evidence of Anchimeric Assistance in the H^- Transfer from 1,1-Dimethylcyclopentane to Alkyl Cations."

J. Phys. Chem., **100**, 8285-8294 (1996). **DOI:** 10.1021/jp952728l

53. B. Chiavarino, M. E. Crestoni, S. Fornarini, D. Kuck
"[Arene · Me_3C^+] non-Covalent Complexes in the Gas Phase (Trifluoro)methylation of Tertbutyl-substituted Diphenylalkanes."
Int. J. Mass Spectrom. Ion Processes, **148**, 215 (1995).

52. B. Chiavarino, M. E. Crestoni, S. Fornarini
"Aromatic Silylation of Trimethylgermylbenzene by Gaseous Me_3Si^+ Ions via Me_3Ge^+ Displacement"
Organometallics, **14**, 2624 (1995).

51. M. Attinà, F. Cacace, S. Fornarini
"$[R_3Si\text{-Arene}]^+$ σ-Complexes in the Gas Phase"
Angew. Chem. Int. Ed. Engl. **34**, 654-655 (1995) DOI: 10.1002/anie.199506541

50. M. E. Crestoni, S. Fornarini, M. Lentini, M. Speranza
"Hydride Ion Transfer Reaction in the Gas Phase. 1. Pressure Dependence of the Reaction Efficiency as a Criterion to Recognize Anchimeric Assistance."
J. Chem. Soc., Chem. Commun., 121-122 (1995).

49. M. E. Crestoni, S. Fornarini, D. Kuck
"Gas-Phase Protonation of α,ω-Diphenylalkanes"
J. Phys. Chem., **99**, 3150-3155 (1995). **DOI:** 10.1021/j100010a027

48. M. E. Crestoni, S. Fornarini, D. Kuck
"Internal Solvation Effects on the Reactivity of α,ω-Diphenylalkanes towards Me_3C^+ Ions."
J. Phys. Chem., **99**, 3144-3149 (1995). **DOI:** 10.1021/j100010a026

47. M. E. Crestoni, S. Fornarini
"Aromatic Alkylation by Gaseous Me_3C^+ Ions. Kinetic Role of Deprotonation of Intermediate Arenium Ions"
J. Am. Chem. Soc., **116**, 5873-5879 (1994). **DOI:** 10.1021/ja00092a043

46. M. E. Crestoni, S. Fornarini
"Long-Lived *ipso*-Silylated *p*-Toluenium Ions: Evidence from a Kinetic Isotope Effect"
Angew. Chem. Int. Ed. Engl., **33**, 1094-1096 (1994). DOI: 10.1002/anie.199410941

45. F. Cacace, M. E. Crestoni, S. Fornarini
"Ion-Molecule Reactions in Gaseous CF_4/CO Mixtures. Formation and Reactivity of CF_3CO^+ Ions"
J. Phys. Chem., **98**, 1641 (1994). 10.1021/j100057a017

44. M. E. Crestoni, S. Fornarini, G. Occhiucci
"Gas Phase Reactivity of Aromatic Silanes. The Reaction of $Ph(CH_2)_xSiMe_3$ (x = 0, 1) with Cationic Electrophiles"
J. Organometal. Chem., **465**, 109 (1994).

43. F. Grandinetti, M. E. Crestoni, S. Fornarini, S. Speranza
"Ionic Lewis Superacids in the Gas Phase. Part 4. CF_3^+ Initiated Ion-Molecule Reaction Patterns in the ?-Radiolysis of CF_4/n-Bases Gaseous Mixtures "
Int. J. Mass Spectrom. Ion Processes, **130**, 207 (1994).

42. F. Grandinetti, G. Occhiucci, M. E. Crestoni, S. Fornarini, M. Speranza
"Ionic Lewis Superacids in the Gas Phase. Part 3. Reactions of Gaseous CF_3^+ with Nitrogen Bases"
Int. J. Mass Spectrom. Ion Processes, **127**, 137 (1993).

41. F. Grandinetti, G. Occhiucci, M. E. Crestoni, S. Fornarini, M. Speranza
"Ionic Lewis Superacids in the Gas Phase. Part 2. Reactions of Gaseous CF_3^+ with Oxygen Bases"
Int. J. Mass Spectrom. Ion Processes, **127**, 123 (1993).

40. C. Galli, S. Fornarini
"Aromatic Acylation in Homogeneous solution and in the Gas Phase: the Mechanistic Relevance of the Mesitylene/durene Reactivity Ratio"
J. Chem. Soc. Perkin Trans. 2, 1147 (1993).

39. F. Cacace, M. E. Crestoni, S. Fornarini, D. Kuck

"Interannular Proton Transfer in Thermal Arenium Ions from the Gas-Phase Alkylation of 1,2-diphenylethane"

J. Am. Chem. Soc., **115**, 1024 (1993).

38. F. Cacace, M. E. Crestoni, S. Fornarini
"Proton Shifts in Gaseous Arenium Ions and Their Role in the Gas-Phase Aromatic Substitution by Free Me_3C^+ and Me_3Si^+ Cations"
J. Am. Chem. Soc., **114**, 6776 (1992).

37. G. Cerichelli, M. E. Crestoni, S. Fornarini
"Brønsted versus Lewis Acid Reactivity of Gaseous Cation ($C_2H_5^+$, i-$C_3H_7^+$, HCO^+) toward Arenes"
J. Am. Chem. Soc., **114**, 2002 (1992).

36. G. de Petris, S. Fornarini, G. Occhiucci
"Protonated Methanesulfonic Acid and Related Ions: a Study of their Gas Phase Structure and Reactivity"
Int. J. Mass Spectrom. Ion Processes, **112**, 231 (1992).

35. F. Cacace, M. E. Crestoni, A. Di Marzio, S. Fornarini
"Gas Phase Aromatic Substitution. Reactivity of α,α,α-trifluoromethoxy)benzene toward Charged Electrophiles"
J. Phys. Chem., **95**, 8731 (1991).

34. S. Fornarini
"Mass Spectra of Amidines and Related Compounds"
in *The Chemistry of Amidines and Related Compounds* Vol. II, Eds.S. Patai, Z. Rappoport, Wiley, New York, 1991.

33. S. Fornarini
"Mass Spectrometry of Sulfonic Acids and their Derivatives"
in *"The Chemistry of Sulfonic Acids Esters and their Derivatives"*, Eds.S. Patai, Z. Rappoport, Wiley, New York, 1991.

32. G. Cerichelli, M. E. Crestoni, S. Fornarini
"The Fluorination of Simple Five-Membered Heteroaromatic Compounds with Elemental Fluorine"
Gazz. Chim. Ital. , **120**, 749 (1990).

31. M. E. Crestoni, S. Fornarini, M. Speranza
"Gas Phase Heteroaromatic Substitution. Silylation of Simple Five-Membered Heteroaromatic Rings by Trimethylsilyl Cations"
J. Am. Chem. Soc., **112**, 6929 (1990).

30. S. Fornarini, M. Speranza
"Vinylation of Aromatic Substrates by Free Unsolvated Vinyl Cation in the Gaseous and Liquid Phase"
J. Am. Chem. Soc., **111**, 7402 (1989).

29. M. E. Crestoni, S. Fornarini
"Direct Fluorination of Thiophene and N-Methylpyrrole"
Gazz. Chim. Ital., **119**, 203 (1989).

28. M. E. Crestoni, S. Fornarini
"Gas-phase Reactions of Charged Electrophiles with Styrene and Phenylacetylene"
J. Am. Chem. Soc., **111**, 6008 (1989).

27. S. Fornarini, V. Muraglia
"Direct Evidence for the Existence and Relative Stability of Gaseous Ethylenebenzenium Ions from a ^{13}C-Labelling Study"
J. Am. Chem. Soc., **111**, 873 (1989).

26. S. Fornarini, M. Speranza
"Arylation of Cyclic Ethers by Gaseous Phenylium Ions. Formation and Behavior of Phenoxenium Ions in the Gas Phase"
Can. J. Chem., 66, 2506 (1988).

25. F. Cacace, M. E. Crestoni, G. de Petris, S. Fornarini, F. Grandinetti
"A Comparative Study of Gas Phase Aromatic Desilylation and Detertbutylation by Charged Electrophiles"
Can. J. Chem., **66**, 3099 (1988).

24. F. Cacace, M. E. Crestoni, S. Fornarini, R. Gabrielli
"Cationic Aromatic Silylation in the Gas Phase"
Int. J. Mass Spectrom. Ion Processes, **84**, 17-32 (1988).

23. S. Fornarini
"Direct Aromatic Substitution by Trimethylsilyl Cations"
J. Org. Chem., **53**, 1314 (1988).

22. S. Fornarini
"Positive Evidence for Tetrahedral R'C(OR)$_3$H$^+$ Intermediates in the Gas Phase"
J. Am. Chem. Soc., **110**, 963 (1988).

21. S. Fornarini, C. Sparapani, M. Speranza
"Gas Phase Acid-Induced Nucleophilic Displacement Reactions. Structural Analysis of Intermediate Ions Formed by the Decomposition of β-Arylethyl Onium Ions"
J. Am. Chem. Soc., **110**, 42 (1988).

20. S. Fornarini, C. Sparapani, M. Speranza
"Gas Phase Acid-Induced Nucleophilic Displacement Reactions. Structural and Stereochemical Evidence for the Existence and Relative Stability of Alkylenebenzenium Ions in the Gas Phase"
J. Am. Chem. Soc., **110**, 34 (1988).

19. B. Aliprandi, F. Cacace, S. Fornarini
"Gas Phase Alkylation of Dihalobenzenes by Free Isopropyl Ions"
Tetrahedron, **43**, 2831 (1987).

18. S. Fornarini, M. Speranza
"Gas Phase Addition of Vinyl Cation to Hydrogen and Methane. A Nuclear Decay Study"
J. Phys. Chem., **91**, 2154 (1987).

17. F. Cacace, G. de Petris, S. Fornarini, P. Giacomello
"Gas Phase Cationic Methylation of Biphenyl and Methylbiphenyls. A Mass Spectrometric and Radiolytic Study"
J. Am. Chem. Soc., **108**, 7495 (1986).

16. S. Fornarini, R. Gabrielli, M. Speranza
"Gas Phase Reactivity of Vinyl Cation towards Simple Molecules. Hydrogen and Methane"
Int. J. Mass Spectrom. Ion Processes, **72**, 137 (1986).

15. S. Fornarini, M. Speranza
"The Gas Phase Reaction of Free Phenylium Ion with 1,3-Butadiene"
Gazz. Chim. Ital., **116**, 341 (1986).

14. S. Fornarini, M. Speranza
"Reaction of Vinyl Cation with Hydrogen and Methane as Studied by FT-MS and Nuclear Decay Methods"
Adv. Mass Spectrom., B, 801 (1985).

13. S. Fornarini, M. Speranza
"Gas Phase Reactions of a Free Vinyl Cation with Benzene and Free Phenylium Ion with Ethylene. A Comparative FT-ICR and Nuclear Decay Study"
J. Am. Chem. Soc., **107**, 5358 (1985).

12. M. Attinà, F. Cacace, G. de Petris, S. Fornarini, P. Giacomello
"Ipso Aromatic Alkylation in the Gas Phase. Intermediacy and Structure of Gaseous Heptaalkylbenzenium Ions"
J. Am. Chem. Soc., **107**, 2297 (1985).

11. S. Fornarini, M. Speranza
"Is Gaseous Phenylium Ion Unreactive toward Acetylene?"
J. Chem. Soc. Chem. Commun., 1692 (1985).

10. S. Fornarini, M. Speranza, M. Attinà, F. Cacace, P. Giacomello
"Gas-Phase Protonation of Allene and Propyne. Remarkably Selective Formation of 2-Propenyl Ions"
J. Am. Chem. Soc., **106**, 2498 (1984).

9. S. Fornarini, M. Speranza
"Tritiated Ethylene as Precursor of Free Vinyl Cation"
Tetrahedron Lett., **25**, 869 (1984).

8. S. Fornarini, M. Speranza
"Arylation of Dialkyl Ethers by Gaseous Phenylium Ions. Formation and Behavior of Dialkylphenyloxonium Ions in the Gas Phase"
J. Chem. Soc., Perkin Trans. 2, 171 (1984).

7. G. Angelini, S. Fornarini, M. Speranza
"A Nuclear Decay Approach to a Complete Characterization of Free Phenylium Ion in the Gaseous and Condensed Phase"
Bull. Soc. Chim. Belg., **91**, 414 (1982).

6. G. Angelini, S. Fornarini, M. Speranza
"Gas and Liquid Phase Reactions of Free Phenylium Cation with Methanol"
J. Am. Chem. Soc., **104**, 4773 (1982).

5. C. F. Bernasconi, S. Fornarini

"Nucleophilic Additions to Olefins. 4. Structure - Reactivity Relationships in the Reactions of Amines with Substituted Benzylidene Meldrum's Acids. Evidence for Intramolecular Proton Transfer to Carbon"

J. Am. Chem. Soc., **102**, 5329 (1980).

4. C. F. Bernasconi, J. P. Fox, S. Fornarini
"Nucleophilic Addition to Activated Olefins. 3. Reactions of Piperidine and Morpholine with Benzylidenemalononitrile in 50% Dimethylsulfoxide - 50% Water. Intrinsic Barriers in Nucleophilic Additions"

J. Am. Chem. Soc., **102**, 2810 (1980).

3. R. Chiarizia, P. R. Danesi, S. Fornarini
"Extraction Kinetics of Iron(III) from Aqueous Nitrate Solutions to Toluene Solutions of Tri-n-butylacetohydroxamic Acid"

J. Inorg. Nucl. Chem., **41**, 1465 (1979).

2. G. Doddi, S. Fornarini, G. Illuminati, F. Stegel
"Rates and Equilibria for the Addition of Methoxide Ion to 2,6-Diphenyl- and 4-Methoxy-2,6-diphenylpyrylium Cations"

J. Org. Chem., **44**, 4496 (1979).

1. S. Bersani, G. Doddi, S. Fornarini, F. Stegel
"Reactions of Heteroaromatic Cations with Nucleophilic Reagents. Addition of Methoxide Ion to 2,6-Diphenyl- and 4-Methoxy-2,6-diphenylpyrylium Cations"

J. Org. Chem., **43**, 4112 (1978).