



# Structure and relative probabilities of formation of chlorobenzene dications induced by electron, proton and photon impact



Sala de conferencias.  
Dpto. Física-UNS.



Viernes 10/11. 15hs.



**Dra. Wania Wolff**

Instituto de Física  
Universidade Federal do Rio de Janeiro

2017

10/11

**M**onochlorobenzene ( $C_6H_5Cl$ ) is proposed as a prototypical molecule for studying substituent effects on the benzene ring, demonstrating the advantages of combining theoretical and experimental techniques to probe the molecular structure and formation. A literature survey has shown limited insights on mono substituted benzene derivatives, especially on the formation of multiply-charged parent ions. In this talk we present the structure and relative stabilities of chlorobenzene dications generated by the multiple ionization of  $C_6H_5Cl$  induced by electron, proton and photon impact. The most stable structure and low-lying isomers of multiply-charged parent ions (dications and trications) are analysed by Generalized Valence Bond and Density Functional Theory calculations, which revealed unusual carbon-chlorine bonding patterns. Experimentally, direct evidence of the formation of stable doubly-charged molecular parent ions observed by time-of-flight mass spectroscopy. Mass spectra and ion yields give the measure of the dications formation and their stability against dissociation is analysed through the ratios of dication to the molecular ion. Both aspects were investigated using keV energetic photons around the chlorine K-edge, electrons with energies from the double ionization threshold to 2000eV and low-energy protons in the 50-155 keV range. From the chemist's point of view, the authors hope that the results presented herein will encourage experimentalists to synthesize novel chlorine-containing species with unusual bonding pattern. Similarly, from the physicist's point of view it is expected that these results will enable investigation into the competition between direct double ionization and auger emission channels in the formation of stable multiply-charged parent ions.



 [www.fisica.uns.edu.ar](http://www.fisica.uns.edu.ar)

 Departamento de Física-UNS