

Electron collisions with phenol: a joint experimental and theoretical investigation

R. F. da Costa¹, E. M. de Oliveira², M. H. F. Bettega³, M. T. do N. Varella⁴, R. F. C. Neves^{5,6,7}, G. B. da Silva^{5,8}, H. V. Duque^{5,6}, M. C. A. Lopes⁶, D. B. Jones⁵, K. L. Nixon⁶, K. Ratnavelu⁹, M. J. Brunger^{5,9}, F. Blanco¹⁰, R. Colmenares¹¹, P. Limão-Vieira¹², G. Garcia¹³, and M. A. P. Lima²

¹Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, 09210-580 Santo André, São Paulo, Brazil

²Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, 13083-859 Campinas, São Paulo, Brazil

³Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, 81531-990 Curitiba, Paraná, Brazil

⁴Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05315-970 São Paulo, São Paulo, Brazil

⁵School of Chemical and Physical Sciences, Flinders University, GPO Box 2100, Adelaide SA 5001, Australia

⁶Departamento de Física, UFJF, Juiz de Fora, Minas Gerais, Brazil

⁷Instituto Federal do Sul de Minas, Campus Poços de Caldas, Minas Gerais, Brazil

⁸Universidade Federal de Mato Grosso, Barra do Garças, Mato Grosso, Brazil

⁹Institute of Mathematical Sciences, University of Malaya, 50603 Kuala Lumpur, Malaysia

¹⁰Departamento de Física Atómica, Molecular y Nuclear, Universidad Complutense de Madrid, Ciudad Universitaria, 2840 Madrid, Spain

¹¹Hospital Ramón y Cajal, 28034 Madrid, Spain

¹²Laboratório de Colisões Atómicas e Moleculares, CEFITEC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal

¹³Instituto de Física Fundamental, CSIC, Serrano 113-bis, 28006 Madrid, Spain

romarly.costa@ufabc.edu.br

It has long been recognized that lignocellulosic biomass is a potential sustainable source of mixed sugars for fermentation to biofuels. During the last decades many technologies have been developed that allow this conversion process to occur and, nowadays, the clear objective is to make the use of such technologies cost-effective. Recently, it has been found that free-electrons and radical species formed within atmospheric plasmas have the ability to overcome the natural resistance of plant cell walls thus allowing for an enhancement of microbial and enzymatic deconstruction [1]. In this context, low-energy electrons which are produced within the plasma environment have the potential to induce breakage of chemical bonds through dissociative electron attachment, electron-impact excitation and other fragmentation processes.

In this work we report a joint experimental and theoretical effort in order to determine reliable elastic and electronically inelastic cross sections for low-energy electron collisions with phenol [2], a key structural subunit of lignin.

References

- [1] N. Schultz-Jensen, F. Leipold, H. Binslev, and A. Thomsen, *Appl. Biochem. Biotechnol.*, **163**, (2011), 558; J. Amorim, C. Oliveira, J. A. Souza-Correa, and M. A. Ridenti, *Plasma Processes Polym.*, **10**, (2013), 670.
- [2] D. B. Jones *et al.*, *J. Chem. Phys.* **141**, (2014), 074314; R. F. da Costa *et al.*, *J. Chem. Phys.*, **142**, (2015), 104304; R. F. C. Neves *et al.*, *J. Chem. Phys.*, **142**, (2015), 104305.