

Electron collisions with phenol: Total, integral, differential, and momentum transfer cross sections and the role of multichannel coupling effects on the elastic channel

R. F. da Costa^{*1}, E. M. de Oliveira[†], M. H. F. Bettega[‡], M. T. do N. Varella[‡], D. B. Jones[§], M. J. Brunger^{§,*}, F. Blanco[‡], R. Colmenares[§], P. Limão-Vieira[‡], G. García[¶] and M. A. P. Lima[†]

^{*} Departamento de Física, Universidade Federal do Espírito Santo, 29075-910, Vitória, Espírito Santo, Brazil

[†] Instituto de Física “Gleb Wataghin”, Universidade Estadual de Campinas, 13083-859,

Campinas, São Paulo, Brazil

[‡] Departamento de Física, Universidade Federal do Paraná, CP 19044, 81531-990, Curitiba, Paraná, Brazil

[‡] Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, São Paulo, Brazil

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

^{*} Institute of Mathematical Sciences, University of Malaya, 50603 Kuala Lumpur, Malaysia

[‡] Departamento de Física Atomica, Molecular y Nuclear, Universidad Complutense de Madrid, Ciudad Universitaria, 2840 Madrid, Spain

[§] Hospital Ramón y Cajal, 28034 Madrid, Spain

[‡] Laboratório de Colisões Atômicas e Moleculares, CEFITEC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal

[¶] Instituto de Física Fundamental, CSIC, Serrano 113-bis, 28006 Madrid, Spain

Synopsis We report theoretical total, integral, differential and momentum transfer cross sections for electron scattering by phenol (C_6H_5OH). The calculated cross sections with two different methodologies, the independent atom method with screening corrected additivity rule (IAM-SCAR), and the Schwinger multichannel method with pseudopotentials (SMCPP).

Lignocellulosic biomass has long been recognized as a potential sustainable source of mixed sugars for fermentation to biofuels. It is now widely accepted that the natural resistance of plant cell walls to microbial and enzymatic deconstruction (collectively known as biomass recalcitrance) is largely responsible for the high cost of lignocellulose conversion. 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 [1]. In this context, low-energy electrons 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 calculated results obtained in a joint experimental and theoretical effort in order to determine reliable cross sections for low-energy electron collisions with phenol [2], a molecule that may be regarded as a key structural subunit of lignin. The SMCPP method in the N_{open} -channel coupling scheme, at the static-exchange-plus-polarization approximation, is employed to calculate the scattering amplitudes at impact energies ranging from 5.0 eV to 50 eV. We discuss the multichannel coupling effects in the calcu-

lated cross sections, in particular how the number of excited states included in the open-channel space impacts upon the convergence of the elastic cross sections at higher collision energies. The IAM-SCAR approach was also used to obtain the elastic differential cross sections (DCSs) and for correcting the experimental total cross sections for the so-called forward angle scattering effect. We found a very good agreement between our SMCPP theoretical differential, integral, and momentum transfer cross sections and experimental data for benzene (a molecule differing from phenol by replacing a hydrogen atom in benzene with a hydroxyl group). Although some discrepancies were found for lower energies, the agreement between the SMCPP data and the DCSs obtained with the IAM-SCAR method improves as the impact energy increases.

References

- [1] J. Amorim *et al.* 2013 *Plasma Processes Polym.* **10** 670; E. M. de Oliveira *et al.* 2013 *Phys. Chem. Chem. Phys.* **15** 1682.
- [2] D. B. Jones *et al.* 2014 *J. Chem. Phys.* **141** 074314; R. F. C. Neves *et al.* 2015 *J. Chem. Phys.* **142** 194302; R. F. da Costa *et al.* 2015 *J. Chem. Phys.* **142** 194304; R. F. C. Neves *et al.* 2015 *J. Chem. Phys.* **142** 194305.

¹E-mail: romarly.costa@ufes.br