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Elastic Scattering of Low-Energy Electron by Lignin Precursors

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Synopsis We present cross sections for electron collisions with monolignol precursors obtained with the Schwinger Multichannel method. For C_s phenol system, π^* resonances are found in the A'' irreducible representation. So, mechanisms for dissociative electron attachment could give rise if σ^* resonances are found in the monolignols.

Replace fossil fuels for biofuels from renewable sources is one way of contributing to reduction of the emission of greenhouse gases. In this scenery, production of ethanol from lignocellulosic biomass plays a very important role. Besides substituting gasoline, cellulosic bioethanol can be a good strategy to combat undesirable increase of both area occupied by sugarcane plantation and burning [1].

Lignocellulosic biomass is a heterogeneous organic polymer that consists of cellulose fibers embedded tightly within hemicellulose and lignin. Due to the complexity structure, it is necessary to submit the biomass to a pretreatment in order to break it down and, consequently, improving the efficiency of enzymatic hydrolysis. This pretreatment may be done through the use of a low-cost atmospheric-pressure plasmas [2], which can generate interesting reactive species for ethanol productions.

Is well known that DNA damage arises from dissociative electron attachment, a mechanism in which electrons are resonantly trapped by DNA subunits [3]. Believing that a similar process can be possible in biomass, theoretical resonance energies can be useful for guide the plasma-based pretreatment to break down linkages of interest in lignocellulosic material.

Aiming at offering theoretical support to this pretreatment, we intend to study the interaction between the low-energy electrons of the plasma and the material under treatment. However, the complexity of biomass structure makes the description of the potential surfaces of the relevant metastable ions very computationally demanding, even for biomass subunits. Since phenol molecule is a precursor of monolignols (lignin units), it can be an interesting prototype to-

wards understanding the dissociation dynamics of biomass.

In this work we present elastic cross sections for electron scattering by phenol molecules (C_s system) obtained with the Schwinger Multichannel method [4]. Our results indicate three π^* shape resonances in the A'' symmetry (see figure). These resonances, together with σ^* ones that can occur in monolignols units, both direct and indirect dissociation mechanisms would be expected during the pretreatment of biomass.

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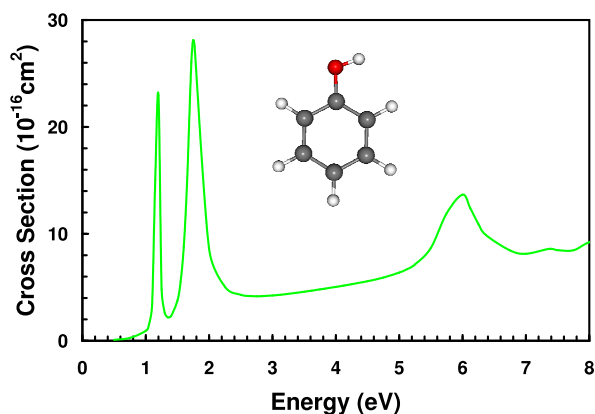


Figure 1. Electron-phenol system: A'' symmetry.

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