

Differential and integral cross sections for electron impact excitation of vibrational and electronic states in phenol

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Synopsis. In this investigation was obtained differential and integral cross sections for electron impact excitation of vibrational and electronic states in phenol. In order to investigate these interactions, experimental electron-energy loss spectra (EELS) were recorded to phenol, measured at impact energies of 15, 20, 30, 40 and 250 eV, for angles between 10° and 90°.

The conversion of lignocellulosic biomass into biofuels is a sustainable source of energy to meet global energy demands. Low-energy electrons in plasmas have the potential to overcome the biomass physicochemical resistance enabling the production of high value chemicals. This happens due to chemical breakdown induced through dissociative electron attachment or electron impact excitation- or ionization-fragmentation processes. In this work was investigated the electron scattering by phenol, a subunit of the lignocellulosic biomass. Experimental electron-energy loss spectra (EELS) were recorded to phenol, measured at impact energies of 15, 20, 30, 40 and 250 eV, for angles between 10° and 90° by recording the number of scattered electrons detected at each energy loss value [1]. EELS have been measured using two different electron scattering spectrometers at low (15-40 eV) or intermediate (250 eV) incident electron energy. Both are based at Flinders University in Adelaide as described in Brunger and Teubner [2]. The energy resolution of the low-energy apparatus is ~80 meV (FWHM), while that for the intermediate-energy apparatus is typically ~1.1 eV (FWHM). A well-collimated electron beam, with a well-defined energy spread, is incident on an orthogonal beam of target molecules. Electrons that scatter from the sample molecules through an angle θ , enter a hemispherical analyser where they are energy analysed. Electrons with the correct scattered energy (E_a) are then detected using a channel-electron multiplier scaler synchronised to a linear voltage ramp that varied the detected energy loss. The EELS were deconvoluted into contributions arising from each individual or unresolved combination of excited states. Gaussian functions were employed to describe the spectral profiles for each resolvable inelastic feature and the elastic scattering peak. These spectra were used to derive

Cross Sections (CS) and Generalized Oscillator Strengths (GOS) for the dipole-allowed electronic transitions, also allowing the determination of their Optical Oscillator Strengths. Differential cross sections (DCS's) were measured for the electron-impact excitation of the electronic states as well as of a number of composite unresolved vibrational modes in phenol [3,4].

These investigations provide the first results published on the literature to singlet and triplet excited electronic states of phenol, up to the first ionization potential and, to the vibrational excitation Cross Sections. In addition, it were obtained integral cross sections (ICS's) data for electron impact vibrational and electronic excitations in phenol [5].

References

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