

Abstract Submitted
for the GEC10 Meeting of
The American Physical Society

Electron-impact collisions with gas-phase thiophene molecules

ROMARLY DA COSTA, Universidade Federal do ABC, MÁRCIO BETTEGA, Universidade Federal do Paraná, MARCO LIMA, Laboratório Nacional de Ciência e Tecnologia do Bioetanol — In this work we report elastic and electronically inelastic cross sections for low-energy electron collisions with thiophene molecules. The scattering amplitudes are obtained using the Schwinger multichannel method implemented with pseudopotentials for energies ranging from 0 to 30 eV. Elastic calculations are performed at the static-exchange and static-exchange plus polarization levels of approximation. Electronic transition from ground state to the 1^3B_2 excited state of thiophene is obtained within a five-channel close-coupling model. The importance of competition among the energetically accessible channels is analyzed by comparing the results obtained at different levels of multichannel close-coupling and the influence of the polarization of the target on the elastic and electronic excitation processes is also investigated through the comparison of calculations performed with and without inclusion of this effect. Preliminary results for integral and momentum transfer elastic cross sections revealed the presence of two shape resonances at around 1 eV and 2.8 eV which are ascribed to the B_1 and A_2 symmetries of the C_{2v} point group, respectively. These results are in very good agreement with available experimental measurements for vertical attachment energies [J. Phys. Chem. A **108**, 5721 (2004)].

Romarly da Costa
Universidade Federal do ABC

Date submitted: 14 Jun 2010

Electronic form version 1.4