SPINFLIP CROSS SECTIONS AND POLARIZATION FRACTION OF CCO RADICAL BY ELECTRON IMPACT

Milton Massumi Fujimoto[1], Sergio Eduardo Michelin[2], and Lee Mu-Tao[3]

1) Departamento de Física, UFPR – Universidade Federal do Paraná, 81531-990 Curitiba, PR, Brasil
2) Departamento de Física, UFSC – Universidade Federal de Santa Catarina, 88040-900 Florianópolis, SC, Brasil
3) Departamento de Física, UFSCar – Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brasil

Recently, we study theoretically the elastic cross sections of CCO radical by electron impact [1]. CCO is an open shell molecule with the ground state configuration $X^3\Sigma^-$ and the electron-radical interaction have two spin specific scattering channels, the doublet and quartet coupling between the scattering electron and the open shell electrons of the target. The results of integral cross section by symmetry shown that for incident electron with π symmetry we observed the existence of the shape resonance locate at around 3 and 4.5 eV corresponding to the quartet and doublet scattering channels. The shift of about 1.4 eV of the shape resonance in CCO is due to the different exchange potential operator used in the doublet- and quartet-coupling scattering calculations.

In this work, we calculate the spin-flip cross sections and the polarization fraction for electron collision with CCO molecules, in the energy range of 1eV up to 10 eV. The molecular wave functions are described at Hartree-Fock level and TZV basis set was used to represent the atomic orbitals. The scattering amplitudes for each channel was calculated using the Schwinger Iterative Method and the collision dynamic is represented for one interaction potential including the static, exchange, correlation and polarization effects. The results shown that the spin-flip cross sections and the polarization fraction are important around the resonance peak and bellow 10 eV. In figure 1, the results to the polarization fraction rotationally unresolved show that the spin-flip effect are more accentuated around of the resonance. We also calculated de spin-flip differential cross section and polarization fraction rotationally resolved for the transitions $j=0\rightarrow j'=0,1$ and 2. Additional results will be presented during the symposium.

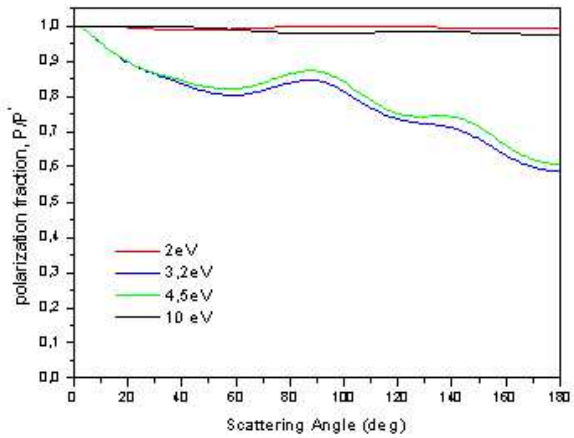

Figure 1: Polarization fraction for the electron scattering by CCO radical.

References

[1] M.M. Fujimoto, M-T. Lee, S. E. Michelin, Phys. Rev. A. **69,** 052706 (2004).

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