Excitation of inner-shell states of C_2H_2 and C_2N_2 polyatomic molecules by electron impact.

S.E. Michelin[†], A.S. Falck[†], M.A. Scopel[†],
J.J. Piacentini[†], H.L. Oliveira[†], K.T. Mazon[†],
A.M.S. Santos[†], M.M. Fujimoto[⋆] and M.-T. Lee[*]

[†] Departamento de Física, UFSC, 88040-900 Florianópolis, SC, Brazil

[*] Departamento de Química, UFSCar, 13565-905, São Carlos, SP, Brazil

[⋆] Departamento de Física, UFPR, 81531-990 Paraná, PR, Brazil

Abstract

Distorted-wave approximation (DWA) is applied to study excitation of core-level electron in C_2H_2 and C_2N_2 polyatomic molecules by electron impact. More specifically, we report calculated differential (DCS) and integral (ICS) cross sections for the $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(1s\sigma_u \rightarrow 1p\pi_g)$and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(1s\sigma_g \rightarrow 1p\pi_g)$ transitions in the C_2H_2 molecule and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_g(2s\sigma_u \rightarrow 2p\pi_u)$and $X\,^1\Sigma_g^+ \rightarrow^{1,3} \Pi_u(2s\sigma_g \rightarrow 2p\pi_u)$ transitions in the C_2N_2 molecule in the 300 - 800 eV incident energy range. The ratios, named RI(3:1), calculated by dividing the distorted-wave integral cross sections(ICS), for transitions leading to the triplet and the singlet core-excited states as a function of incident energy are also reported. The present study shows the RI(3:1) behavior for the C 1s $\rightarrow \pi^*$ transition in each species here studied. The generalized oscillator strength(GOS) profiles for discrete C 1s excited states of C_2H_2 and C_2N_2 have also been calculated, and are compared with the available data reported in the literature. Quantitative agreement between the present theory and experiments is also satisfactory.