Electronic Excitation of Thiophene by Electron Impact

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The seminal work by Boudaïffa et al. [B. Boudaïffa, P. Cloutier, D. Hunting, M. A. Huels, and L. Sanche, Science 287 (2000)] has demonstrated that secondary low-energy electrons can lead to the formation of single- and double strand-breaks in DNA. Since then, the study of electron induced damage to complex biomolecules (basic components of DNA, amino acids) as well as to prototypical molecules (systems carrying out structural and/or functional properties similar to those of DNA components) has been drawn considerable attention. In this work we report on integral and differential cross sections for elastic and electronically inelastic collisions with thiophene (C₄H₄S) molecules. Our calculations were performed with the Schwinger multichannel method (SMC) implemented with pseudopotentials [M. H. F. Bettega, L. G. Ferreira, and M. A. P. Lima, Phys. Rev. A 47 (1993)] and the composition of the space of coupled states was carried out according to the minimal orbital basis for the single configuration interactions (MOB-SCI) strategy [R. F. da Costa, F. J. da Paixão, and M. A. P. Lima, J. Phys. B 38 (2005)]. Elastic calculations were performed in the static-exchange (SE) and static-exchange plus polarization (SEP) approximations for energies ranging from 0 to 15 eV. Inelastic calculations were performed within an up to seven-channel close-coupling level of approximation for energies in the range going from the threshold of the first triplet state (around 3.4 eV) to 15 eV. Our elastic cross sections revealed the presence of two $\pi^*$ shape resonances in the $B_1$ and $A_2$ and also a shape resonance of $\sigma^*$ character, in agreement with previous results available in the literature.