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Ionization of small molecules by electron impact: a Sturmian approach.[1] LORENZO UGO ANCARANI, CARLOS GRANADOS, Universite de Lorraine — The Sturmian approach [1], using Generalized Sturmian Functions (GSF), has been applied successfully to study (e,3e) and (γ,2e) processes in helium. A first extension of the method to molecular systems has been developed for the study of single photoionization [2,3]. In this contribution, we use the tool to look at ionization by electron impact of small molecules. In particular, we are interested in (e,2e) processes on CH_4, NH_3 and H_2O under sufficiently asymmetrical kinematical conditions as to ignore exchange between the two escaping electrons. Within a single active electron approximation, we solve the time-independent, first-order perturbative, Schrödinger equation, expanding the scattering wave function in a GSFs basis set. The adequate asymptotic behavior of all basis elements allows us to extract the transition amplitudes directly from the expansion coefficients, without requiring any evaluation of a matrix element. From the amplitudes, we calculate triply differential cross sections (TDCSs) and compare them with theoretical and relative experimental data. [1] G. Gasaneo et al, Adv. Quantum Chem. 57, 153 (2013). [2] C. M. Granados–Castro et al, Adv.Quantum Chem. 73, 3 (2016). [3] C. M. Granados-Castro, Ph.D. thesis, Université de Lorraine, Metz (2016).

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