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Electron impact single ionization of ammonia. LORENZO UGO ANCARANI, Universite de Lorraine, Metz, France, CARLOS MARIO GRANADOS-CASTRO, Martin-Luther-Universitat Halle-Wittenberg, Germany, ALESSANDRO GENONI, Universite de Lorraine, Metz, France — Recent (e,2e) measurements on polyatomic molecules motivated the development of theoretical methods to calculate and describe ionization cross sections in their most differential form. In this contribution, we study the electron impact single ionization of the outer valence orbital $3a_1$ of NH_3 . In a one-active electron approach, we use Generalized Sturmian Functions (GSF) [1] to expand the scattering wave function; having an appropriate asymptotic outgoing-type behavior, the basis functions are particularly efficient and allow the scattering amplitude to be extracted directly from the asymptotic behavior of the scattering solution (essentially the expansion coefficients) without the need of calculating a transition matrix element. To describe the initial state wave function, we use either the one-center wave function calculated by Moccia [2], or the one obtained by a DFT calculation. The molecular potential is either the one obtained through a static exchange approximation or the one of the DFT approach. The comparison between the two allows us to separate out the importance of the molecular structure quality from the numerical description of the molecular single continuum. We also compare our triple differential cross sections (TDCS) with the recent measurements [3]. [1] C. M. Granados-Castro and L. U. Ancarani, *Eur. J. Phys. D* 71, 65 (2017). [2] R. Moccia, *J. Chem. Phys.* 40, 2176 (1964). [3] R. El Mir et al., *J. Phys. B* 48, 175202 (2015).

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