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Ionization of NH_3 by Electron and Photon Impact

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Ionization of NH_3 by Electron and Photon Impact

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Synopsis We study single ionization by electron and photon impact from the outer valence orbital $3a_1$ of NH_3. The wave function describing the ejected electron is expanded in an appropriate set of Generalized Sturmian Functions. The cross sections obtained with two different molecular target descriptions are compared with each other, and with experimental data.

Photoionization and ionization by electron impact are two fundamental processes which test our ability to describe the target electronic structure, the role of electron-electron interactions and the collision mechanisms. Thanks to diverse experimental and theoretical advances, in the last years the focus on molecular targets has grown. Most of the theoretical studies, however, have been limited to small molecules such as H_2 or N_2. The extension to molecules of traditional atomic approaches is limited by the complexity of the problem (multicenter formulation and generally highly noncentral). Recent $(e,2e)$ measurements on polyatomic molecules motivated the development of theoretical methods to describe ionization cross sections in their most differential form.

We propose to use the Sturmian approach, using generalized Sturmian functions (GSFs) [1] to study single ionization of molecules. The method was applied successfully to study single photoionization of atoms and small molecules [2, 3], as well as double ionization of atoms induced by photon [4], electron [5] or proton [6] impact. In the present investigation, in a one-active electron approach, the scattering wave function is expanded in a set of GSFs that have an appropriate asymptotic outgoing-type behavior; this property makes the method rather efficient. Moreover, the scattering amplitude can be extracted from the asymptotic behavior of the scattering solution (essentially the expansion coefficients), without the need of calculating a transition matrix element.

We study single ionization by electron and photon impact from the outer valence orbital $3a_1$ of NH_3. To describe the initial state wave function, we use either the one-center wave function calculated by Moccia [7], or the one obtained by a DFT calculation. The molecular potential is either the one obtained through a static exchange approximation [8] or the one of the DFT results. 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.

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We compare our results with experimental data. For photoionization we compare with the cross section reported in Ref. [9], while for electron impact we focus on triple differential cross sections (TDCS) and compare with the measurements presented in Ref. [10]; an example is shown in Fig. 1.

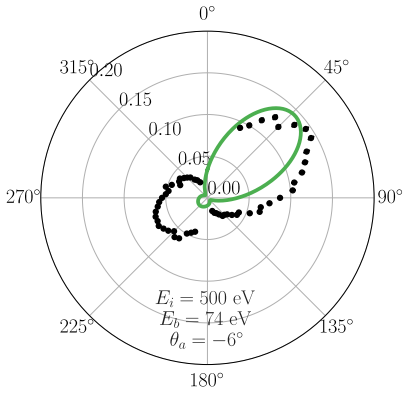

Figure 1. TDCS for $NH_3\left(3a_1^{-1}\right)$. The kinematic conditions are: incident electron energy $E_i = 500$ eV, ejected electron $E_b = 74$ eV. The scattered electron is detected at $\theta_a = -6°$. Experimental data from [10].

References

[1] D. M. Mitnik *et al.* 2011 *Comp. Phys. Commun.* **182** 1145; G. Gasaneo *et al.* 2013 *Adv. Quantum Chem.* **67** 153
[2] C. M. Granados–Castro *et al.* 2016 *Adv. Quantum Chem.* **73** 3
[3] C. M. Granados–Castro 2016 Ph.D. thesis, Université de Lorraine, Metz
[4] J. M. Randazzo *et al.* 2015 *Eur. Phys. J. D* **69** 189
[5] M. J. Ambrosio *et al.* 2015 *J. Phys. B: At. Mol. Opt. Phys.* **48** 055204
[6] M. J. Ambrosio *et al.* 2015 *Phys. Rev. A* **92** 042704
[7] R. Moccia 1964 *J. Chem. Phys.* **40** 2176
[8] L. Fernández–Menchero and S. Otranto 2010 *J. Chem. Phys.* **82** 22712
[9] M. S. Banna *et al.* 1987 *Chem. Phys.* **114** 157
[10] R. El Mir *et al.* 2015 *J. Phys. B: At. Mol. Opt. Phys.* **48** 175202