

Double differential cross sections for ionization of water molecules by ion impact

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Abstract

Single ionization from water molecules by impact of bare ions is studied. Different approximations are employed, within the post and prior versions of the continuum distorted wave–eikonal initial state model, to calculate double differential cross sections. Post–prior discrepancies are observed between theoretical results. The sensitivity of the calculations to the description of the initial bound orbitals is investigated.

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1. Introduction

Single ionization from water molecules by impact of bare ions is studied. We investigate the role played by the representation of the initial bound state of the emitted electron. Two different approaches are considered within the continuum distorted wave–eikonal initial state (CDW–EIS) model: the complete neglect of differential orbitals (CNDO) [1, 2] and the description given by Moccia [3–5] for the ground state of AH_n -type molecules. In the former, each molecular orbital in the initial channel is written as a linear combination of atomic orbitals of the atomic constituents of the molecule. In the latter, the molecular wavefunction is expressed as a weighted sum of Slater-type functions all centred in the heaviest nucleus of the target. Atomic units are used, except when otherwise stated.

2. Theory

We consider the impinging of a bare ion on water molecules. As we study high enough impact energies, we assume that the molecular nuclei remain fixed in their initial positions during the collision. The multielectron problem is reduced to the analysis of a one-active electron system where the active electron is the one to be ionized [6].

Double-differential cross sections (DDCS) as a function of the energy and solid angle of the emitted electron are calculated into their post and prior versions, where the perturbation potential acts on the final and on the initial wavefunctions, respectively. Within the CDW–EIS framework, initial and final distorted wavefunctions χ_i^+ and χ_f^- are described as

$$\chi_i^{+,EIS}(\vec{r}, t) = \varphi_i(\vec{r}) \exp(-i \varepsilon_i t) \mathcal{L}_i^{+,EIS}(\vec{s}), \quad (1)$$

$$\chi_f^{-,CDW}(\vec{r}, t) = \varphi_f(\vec{r}) \exp\left(-i \frac{k^2}{2} t\right) \mathcal{L}_f^{-,CDW}(\vec{s}), \quad (2)$$

respectively, where ε_i is the initial orbital energy, k is the magnitude of the momentum \vec{k} of the ionized electron, and \vec{s} and \vec{r} represent the electron position with respect to the projectile and to the atom where the initial molecular wavefunction is centred, respectively. $\mathcal{L}_i^{+,EIS}$ and $\mathcal{L}_f^{-,CDW}$ are eikonal and Coulomb continuum distortion factors, respectively. The target bound state φ_i of the active electron in the entrance channel is described by the CNDO or the Moccia approximations. In both cases, the target continuum wavefunction φ_f of the electron in the exit channel is considered as a Coulomb one with an effective target charge Z_T^{eff} . It can be defined as an asymptotic charge ($Z_T^{\text{eff}} = 1$) or following the Belkić prescription $Z_T^{\text{eff}} = (-2n^2\varepsilon_i)^{1/2}$. In the

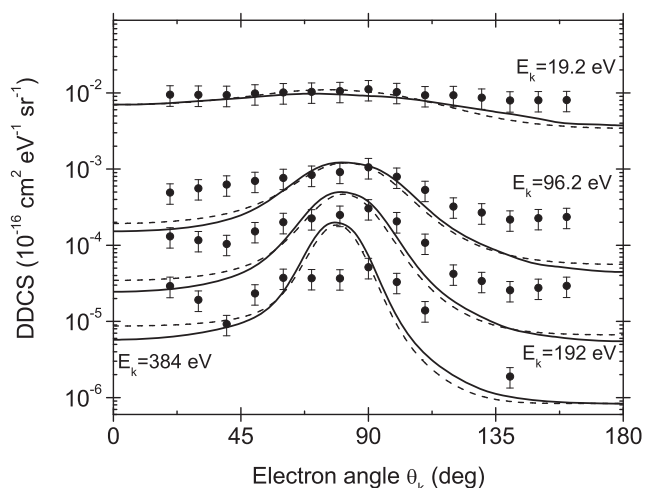


Figure 1. Post-DDCS for C^{6+} at 6 MeV u^{-1} . Results for Moccia (solid line) and CNDO (dashed line) description. Experiments (circles) from [7].

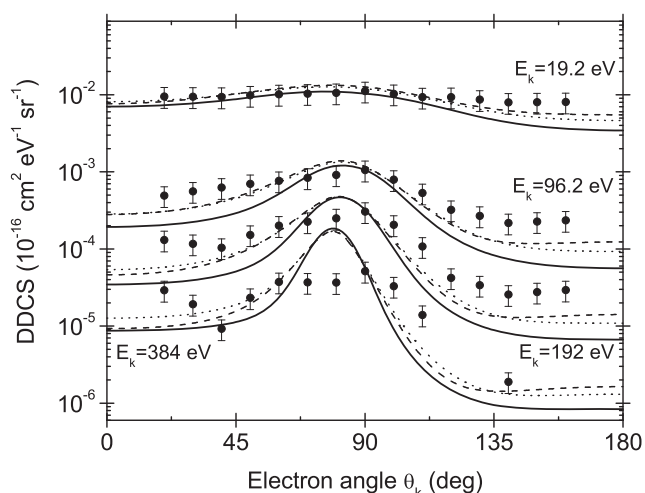


Figure 2. CNDO DDCS for C^{6+} at 6 MeV u^{-1} . Post- with Z_T^{eff} given by Belkić, solid line. Prior- with $Z_T^{\text{eff}} = 1$, dashed line; prior- with Z_T^{eff} given by Belkić, dotted line. Experiments (circles) from [7].

latter one, the n value can be set as the principal quantum number of each atomic orbital for CNDO calculation or can be chosen as the one of the atomic orbital contributing most in the case of Moccia's description.

3. Results and discussion

Our DDCS averaged for all molecular orientations for single ionization of H_2O by impact of C^{6+} at 6 MeV u^{-1} as a function of the emission angle θ_k and for fixed values of the electron energy ε_k are shown in figures 1 and 2 together with experiments [7]. In figure 1, post-DDCS calculated within the CNDO and Moccia representation are plotted, both using the Belkić prescription. For forward emission,

CNDO results are in general larger than the Moccia ones but their differences are smaller as the energy of the emitted electron decreases. For backward angles, the situation is reversed. The same behaviour is observed in the case of proton impact at 500 keV (not shown here). In figure 2, it is observed that CNDO prior-DDCS exhibit better agreement with experiments than the post ones, indicating clear evidence of post-prior discrepancies [8]. This better agreement is due to the fact that within the prior version the interaction between the passive-electron distribution and the active one is included via the initial bound wavefunction whereas in the post version this potential is approximated by an effective Coulomb one. The same effect has been observed in atomic targets, e.g. Ar and Ne, and simple molecules; these results are to be published in a forthcoming paper. Moreover, calculations obtained using $Z_T^{\text{eff}} = 1$ exhibit the same trend but for the highest emission energy considered at forward ejection angles where a weaker influence of the structure of the residual target is expected.

4. Conclusions

Post- and prior-DDCS for impact of C^{6+} at 6 MeV u^{-1} on water molecules have been calculated considering two monocentric approaches (CNDO and Moccia's one) for the initial bound wavefunction of the active electron. Small differences are observed between the post-DDCS calculated with the approximations mentioned above. In consequence, it can be said that post-DDCS are not too sensitive to the choice of the electron initial bound wavefunction. Moreover, discrepancies between CNDO post- and prior-DDCS exist.

This analysis will be applied in the near future to other molecules with strong monocentric character, namely CH_4 and NH_3 .

Acknowledgments

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References

- [1] Senger B and Rechenmann R 1984 *Nucl. Instrum. Methods B* **2** 204
- [2] Senger B 1988 *Z. Phys. D* **9** 79
- [3] Moccia R 1964 *J. Chem. Phys.* **40** 2164
- [4] Moccia R 1964 *J. Chem. Phys.* **40** 2176
- [5] Moccia R 1964 *J. Chem. Phys.* **40** 2186
- [6] Fainstein P D, Ponce V H and Rivarola R D 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 287
- [7] Dal Capello C, Champion C, Boudrioua O, Lekadir H, Sato Y and Ohsawa D 2009 *Nucl. Instrum. Methods B* **267** 781
- [8] Monti J M, Tachino C A, Hanssen J, Fojón O A, Galassi M E, Champion C and Rivarola R D 2013 *Appl. Radiat. Isotopes*, at press

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