

1P015 Extending electron momentum spectroscopy to study the double ionization of water

(IMRAM, Tohoku University) OD. B. Jones, M. Yamazaki, N. Watanabe, M. Takahashi

[Introduction] Water (H_2O) is a major constituent in living organisms and makes up a vast proportion of the Earth's surface. An understanding of its structure and interactions are therefore important in understanding its behaviour in biological systems as well as our own and other planetary atmospheres. Double ionization (DI) processes are of considerable interest to many fields due to the governing role of electron-electron correlations in a wide range of mechanisms. However in the case of water, whilst substantial knowledge has been gained regarding single ionization processes and the resultant cations produced, the structure and behaviour of the dication is considerably less well understood [1].

The binary ($e,2e$) or electron momentum spectroscopy (EMS) technique has long been established as a sensitive probe of molecular structure [2,3]. This technique, which has traditionally been employed to study single ionization mechanisms, has recently been extended to consider the double ionization of helium through an ($e,3-1e$) method [4,5]. Here an electron impact double ionization experiment is performed with the energy and momentum of two fast outgoing electrons being detected in coincidence. Through the conservation of energy and momentum this ($e,3-1e$) method is sensitive to the energy and momentum remaining with the dication and undetected electron. This ($e,3-1e$) experimental method has been identified as an intermediate method lying between EMS and full ($e,3e$) momentum spectroscopy experiments, which suffer from extremely low count rates as they require three outgoing electrons to be detected in coincidence. In the absence of two-step processes, the experimental ($e,3-1e$) cross section is directly proportional to the projection of the ground state on the continuum Coulomb state averaged over initial molecular rotations and outgoing electron directions [6].

[Experimental] We have performed an ($e,3-1e$) experiment to examine the double ionization of water. The experiment has been conducted in the symmetric non-coplanar EMS geometry in an apparatus that has been described previously [7]. Here an incident electron energy of 2055 eV is used, whilst the two fast outgoing electrons are detected in coincidence after undergoing energy and momentum dispersion in a spherical analyser having a mean pass energy of 1000 eV. This allows the measured spectra to be obtained over the binding energy range of 0-100 eV. The present experimental technique yields the simultaneous detection of both the traditional ($e,2e$) events and the double ionization ($e,3-1e$) events. It is noted that this allows the intensity of double ionization events to be directly compared against the intensity of the outer-valence ($e,2e$) events.

[Results and Discussions] A representative example of the observed binding energy spectra summed over the measured azimuthal angles is presented in figure 1. Here it is noted that whilst the double ionization onset is 34 eV [1], the onset of DI is somewhat masked by a breakdown of the molecular orbital picture for the $2a_1$ orbital [8]. However, we highlight the spectral feature observed at ~ 57 eV that is prominent above the continuum and is associated with the opening of additional double ionization channels.

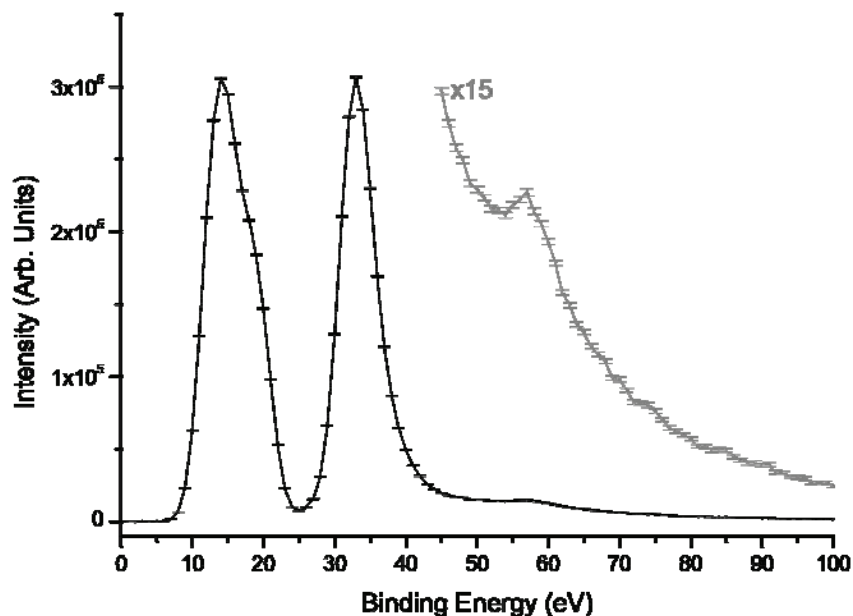


Figure 1: A representative example of the binding energy spectrum of water containing traditional (e,2e) and (e,3-1e) double ionization events.

To our knowledge, this experiment represents the first time that (e,3-1e) momentum spectroscopy for a molecular target has been explicitly considered. The present experimental results therefore represent an important test of theoretical models of double ionization, which have most recently been used to calculate the full (e,3e) five fold differential cross section under a different set of kinematical conditions [9]. The experimental double ionization onsets are also directly comparable to those predicted theoretically.

[References]

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