Journal of Physics: Conference Series **635** (2015) 072042 doi:10.1088/1742-6596/635/7/072042

Cross sections for electron collisions with H_2O: elastic scattering and electronic excitation for the $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ states

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Synopsis We report absolute differential cross sections (DCSs) and integral cross sections (ICSs) for the electronic excitation to the $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ states as well as the elastic scattering of H_2O molecules. The measurements are performed in the scattering angle range of 10 – 130°, and impact energies 15, 20, 30 eV for the electronic excitations and energy range 2.0 – 100 eV for the elastic scattering, respectively.

Electron impact excitation of water molecules is of particular relevance to radiation-driven chemistry in biological systems because several of the lowest-lying states are strongly dissociative, producing H atoms and OH radicals [1]. Itikawa and Mason noted in their review [2] that the angular differential cross sections (DCSs) and angular integral cross sections (ICSs) data for excitation of water by low-energy electron impact were poorly characterized. Therefore, in contrast to the elastic scattering, vibrational and rotational excitation, they were unable to recommend a cross sectional dataset for electronic excitation. Recently, the DCSs for electronic excitation to the $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ lowest-lying states, which correspond to the $1b_1$ to $4a_1$ transitions, have been reported by two different research groups [1, 3]. However, these results have shown serious discrepancies in the angular distributions of the electronic excitation cross sections of these lowest-lying states below 20 eV impact energy. In the present work, in order to fully address this discrepancy, we have performed comprehensive quantitative measurements of the electronic excitation cross sections at impact energy of 15, 20, 30 eV. In addition, we also report cross sections for elastic scattering from water molecules in the energy range of 2.0 – 100 eV.

The present measurements have been carried out using an original crossed-beam electron spectrometer described in detail many times before, see e.g. ref. [4]. Briefly, this spectrometer contains the hemispherical electrostatic monochromator and the analyzer pumped differentially, with virtual apertures, and a series of electron-lens systems to transport and focus the electron beam controlled by computer-driven voltages. The spectrometer was operated at fixed incident electron energy and over the scattered electron angular range of 15° to 130°. The energy resolution was typically 55 - 60 meV (FWHM). A transmission efficiency of the electrostatic analyzer has been decided most carefully and the absolute scale has been obtained by the standard relative flow technique using the well-known elastic DCSs of helium as the reference species. The H_2O sample was obtained from the vapour of ultra-pure water supplied by Wako Pure Chemical Industries, Ltd. The liquid sample was purified to remove dissolved gases by a repeated freeze-pump-thaw procedure. The molecular beam was produced effusively, kept at slightly elevated temperatures (~80° C) throughout the measurements.

In the present measurements, for the DCSs for electronic excitation to the $\tilde{a}^3B_1$ and $\tilde{A}^1B_1$ states, our present measurements and those of Ralphs *et al* [1] are generally consistent, but for the $\tilde{A}^1B_1$ state, we observed quantitative difference at the impact energy of 15 eV. The agreement between the present elastic DCSs and those of Nishimura and Danjo [5] is found to be good in all range of impact energies.

Further details of the results will be presented at the conference.

References

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