Nuclear Motion in the Core-Excited States of H_2O Probed by Sub-Natural-Linewidth Resonant Auger Spectroscopy

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The O 1s photoexcitation spectra of H_2O exhibit two dominant peaks below threshold. The broad structureless peak at 534 eV corresponds to the O1s $\rightarrow 4a_1$ excitation,whereas the peak with partially resolved vibrational structure at 536 eV is assigned to O1s $\rightarrow 2b_2$. We have investigated nuclear motions in the O $1s^{-1}4a_1$ and $1s^{-1}2b_2$ excited states using resonant Auger spectroscopy. The experiment was carried out on beamline 27SUat SPring-8.The electron spectra were collected with a high-resolution electron spectrometer SES-2002 (Gammadata-Scienta) under sub-natural-linewidth conditions, i.e.with overall width (< 100 meV) smaller than the lifetime broadening of the core-excited states (~150 meV).

.The resonance enhancement of photoemission intensity from the $1b_1$ and $1b_2$ orbitals are significant. The progression of the symmetric stretching vibrations is clearly seen in the $1b_1$ photoemission band, whereas the vibrational members are only partially resolved in the $1b_2$ photoemission band because of overlap between bending and stretching modes. It is interesting to notice that the relative intensity of the symmetric stretching mode versus the bending mode changes as a function of photon energy, .e. when different portions of the potential surface of the intermediate state are sampled. Note also that the population of high vibrational members increases with the increase in the vibrational energy in the core-excited state. The reason why vibrations are highly excited in the Auger final state is that the core-excited state is unstable at the stable point of the ground state along the stretching and

bending coordinates. Therefore nuclear motions along these coordinates proceed in the core-excited state before they are transferred to the Auger final state.

This experiment was carried out with the approval of the SPring-8 program advisory committee and supported in part by Grants-in-Aid for Scientific Research from the Japan Society for the Promotion of Science and by Matsuo Foundation.We are grateful to the staff at SPring-8 for their help.