X-RAY SPECTROSCOPY OF THE LIQUID WATER SURFACE

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The molecular structure of liquid surfaces is a topic of much current interest relevant to problems in many disciplines. We present results from novel studies of liquid water microjets by a variety of spectroscopic methods. Soft X-ray absorption spectroscopy near the oxygen K-edge (530 eV) reveals a fine-structure pattern similar to that found for gaseous water monomers when the surface-selective total ion yield (TIY) is measured, but shows a broadened and blue-shifted spectrum when detecting the bulk-sensitive total electron yield (TEY). An analysis of the TIY EXAFS spectra provide evidence for a lengthening of the nearest neighbor O-O distance at the liquid water jet interface. Fourier Transform infrared microscopy measurements reveal a prominent free O-H stretching resonance and a strongly red-shift ”liquid band” when observing tangent to the microjet axis, but show a typical bulk water band at normal incidence. These results evidence a liquid water surface largely terminated by free OH bonds, and dominated by water molecules interacting at longer distances and with lower coordination number than in the bulk, thus supporting conclusions reached from computer simulations.