High-resolution pulsed-field-ionization zero-kinetic-energy photoelectron spectroscopic study of water

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1 Abstract

H_2O^+ and its isotopologues are molecules subject to the Renner-Teller effect. In the linear configuration, the ground $^2\Pi_u$ electronic state is degenerate, giving rise to the $\tilde{X}^+\ ^2B_1$ and $\tilde{A}^+\ ^2A_1$ states in the bent configuration. Jet-cooled rotationally resolved photoelectron spectra near the origin of the photoionizing transitions, $\tilde{X}^+ \leftarrow \tilde{X}$ of D_2O^+ and HDO^+, and $\tilde{A}^+ \leftarrow \tilde{X}$ of H_2O^+ following single photon ionization have been recorded.
For the $\tilde{X}^+ \leftarrow \tilde{X}$ transition, the analysis of the rotational structure of the origin band (v_1^+ =0, v_2^+ =0, v_3^+ =0) $\leftarrow$ (v_1 =0, v_2 =0, v_3 =0) and of the transitions to the (0,1,0), (0,2,0) and (1,0,0) levels of D_2O^+ and the first excited level of the O-D stretching mode of HDO^+ provided new information on the energy level structure of HDO^+ and D_2O^+ cations and on the photoionization dynamics of water.
For the $\tilde{A}^+ \leftarrow \tilde{X}$ transition, the sensitivity and the high resolution of PFI-ZEKE photoelectron spectroscopy allowed us to observe the rotational structure of low bending vibrational levels of the $\tilde{A}^+\ ^2A_1$ state despite unfavourable Franck-Condon factors. From our experiments we reconstructed the vibrational energy-level structure of H_2O^+ with $v^+_{2,\mathrm{linear}}$ in the range 1-8. These results will be compared with previous ab initio calculations [1] and spectroscopic measurements on levels with $v^+_{2,\mathrm{linear}}$ in the range 6-8 [2,3,4].

References

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