ZEKE-PFI SPECTROSCOPY OF THE Al-(H_2O) AND Al-(D_2O) COMPLEXES.

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The weakly bound complexes Al-(H_2O) and Al-(D_2O) are prepared with pulsed laser vaporization and studied with single-photon ZEKE-PFI spectroscopy. The spectra consist of progressions in the Al-water stretch in the ground state of the corresponding cations (Al-(H_2O): ω_e^+ =327.5 cm^{-1}). The origin energy, Al atom ionization potential and the known Al^+-(H_2O) bond energy produce a neutral Al-(H_2O) bond energy of D_0 = 1440 cm^{-1}. Partially resolved rotational structure suggests that the cation complexes have C_{2v} structures, while the neutrals are non-planar. The neutral structure and energetics are consistent with a metal-water coordinate-covalent bond, which has been predicted by theory.