ASYMMETRY OF M\(^+\)(H\(_2\)O)RG COMPLEXES, (M=V, Nb) REVEALED WITH INFRARED SPECTROSCOPY

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M\(^+\)(H\(_2\)O)Ar and M\(^+\)(H\(_2\)O)Ne clusters (M=V, Nb) were produced in a laser vaporization/pulsed nozzle source. The clusters were then mass selected in a time-of-flight mass spectrometer and studied with infrared photodissociation spectroscopy in the OH stretching region. Spectra showed two bands, with the asymmetric band showing k-type rotational structure. Previous work has shown that most metal-water rare gas-tagged systems adopt C\(_{2v}\) geometry and exhibit the well-known 3:1 ortho:para ratio in the k-type rotational structure in asymmetric stretch band. However these two metals display a pattern that indicates a breaking of the C\(_{2v}\) symmetry. Computational work confirms the breaking of C\(_{2v}\) symmetry giving an Ar-M\(^+\)-O angle of 163.7 degrees for V and 172.1 degrees for Nb. In the ground state we obtain rotational constants that match up well with obtained spectra using 166 degrees for V and 175 degrees for Nb.