

ASYMMETRY OF $M^+(H_2O)RG$ COMPLEXES, ($M=V, Nb$) REVEALED WITH INFRARED SPECTROSCOPY

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$M^+(H_2O)Ar$ and $M^+(H_2O)Ne$ 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.