INFRARED SPECTROSCOPIC INVESTIGATION OF MAGIC NUMBER HYDRATED METAL ION CLUSTERS

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Magic number clusters are clusters that appear with anomalously large intensity compared to their neighbors in mass spectra. Experimental and computational studies of magic number clusters have gained much attention in recent years. The prevailing hypothesis of the origin of the magic numbers is that the clusters form 3D nanoscale cages where all the waters are three or four-coordinated. In order to determine the importance of having only three or four-coordinated waters, we have performed infrared predissociation (IRPD) spectroscopic experiments in the free OH region of water. We investigated the magic number $M^+(H_2O)_{20}$ clusters, where M=Cs, K, H_3O. These spectra are compared with spectra of non-magic clusters and anti-magic clusters. We found evidence of two-coordinated waters in magic number clusters. These results indicate that the formation of a nanoscale water cage is not an important factor in the origin of magic numbers.