EXPLORING THE FRONTIERS OF RARE GAS REACTIVITY: EXPERIMENTAL AND COMPUTATIONAL CHARACTERIZATION OF HArF AND HKrF

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Chemical reactivity of rare gases constitutes a challenging problem for experimentalists and theoreticians. Today, a large number of Xe-containing compounds is known but the chemistry of lighter rare gases is very limited.[1] It has been predicted computationally, that HRgF compounds could be stable for Rg=Rn, Xe, Kr, Ar, He.[2] In this report we describe the experimental preparation and characterization of HArF [3,4] and HKrF. These compounds are prepared in Ar and Kr matrixes via VUV photolysis of HF at 7 K, and subsequent thermal mobilization of H and F atoms. The compounds are identified by IR spectroscopy. The observed spectra are in a good accordance with the ab initio results. Both covalent and ionic interactions contribute to their bonding. Both compounds are formed in two sites and the large spectral shift between the different sites shows strong interaction with the environment. Upon annealing the matrix the less stable site disappears but the lower energy site is stable up to the sublimation temperature of the matrix. This finding is in accordance with the computational results and supports the intrinsic stability of the HRgF molecules. The photodissociation cross section of HKrF and HArF is measured and compared with HKrCl giving information on their excited states.

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