THE SEARCH FOR AN OBSERVABLE HELIUM COMPLEX

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Calculations on the He$\cdots$MX, Ne$\cdots$MX, and Ar$\cdots$MX (M = Cu, Ag, Au; X = F, Cl) complexes at the CCSD and CCSD(T) levels of theory have been conducted.[a]. The RG$\cdots$MX (RG = He, Ne, and Ar) dissociation energies for these complexes have been evaluated by extrapolation to the complete basis set limit. The dissociation energies determined for the He$\cdots$CuF and He$\cdots$AuF complexes have been found to be significant, at $\approx$26 kJ mol^{-1}. The nature of the interactions present in these species have been investigated employing atoms-in-molecules (AIM) analysis, natural bond order analysis, and through evaluation of the dipole/induced dipole and ion/induced dipole interactions. This analysis has shown that the bonding in the strongly bound He$\cdots$CuF and He$\cdots$AuF complexes is slightly covalent in nature.

[a] C. J. Evans, T. G. Wright and A. M. Gardner, *J. Phys. Chem. A*, 114, 4446, (2010)