THE SEARCH FOR AN OBSERVABLE HELIUM COMPLEX

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Calculations on the He···MX, Ne···MX, and Ar···MX (M = Cu, Ag, Au; X = F, Cl) complexes at the CCSD and CCSD(T) levels of theory have been conducted.[a]. The RG···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···CuF and He···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···CuF and He···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)