COUPLED CLUSTER CALCULATIONS FOR COMPLEXES BETWEEN AN ARGON ATOM AND A LINEAR MOLECULE OR CATION

PETER BOTSCHWINA and RAINER OSWALD, *Institut für Physikalische Chemie, Universität Göttingen, Tammanstraße 6, D-37077 Göttingen, Germany*.

Geometric structures and various spectroscopic properties were calculated by the coupled cluster variant CCSD(T) for a number of complexes between an argon atom and linear neutral molecules (HCCH, HC_3N and HC_4H) and cations ($HCNH^+$, $HCCH^+$, HC_3NH^+ and HC_4H^+). The electronic ground state of $Ar\cdots HCCH^+$ has $^2A_1$ symmetry with a T shaped equilibrium structure. The linear form of $Ar\cdots HC_4H^+$ is energetically favoured over the T form, while the opposite holds for the corresponding neutral complex.