

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

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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, HC₃N and HC₄H) and cations (HCNH⁺, HCCH⁺, HC₃NH⁺ and HC₄H⁺). The electronic ground state of Ar · · HCCH⁺ has ²A₁ symmetry with a T shaped equilibrium structure. The linear form of Ar · · HC₄H⁺ is energetically favoured over the T form, while the opposite holds for the corresponding neutral complex.