AB INITIO TEST STUDY ON THE VERTICAL EXCITATION ENERGY OF COAr

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Accurate ab initio potential energy surfaces in the framework of the supermolecule approach are obtained using high-level ab initio methods of quantum chemistry. They are developed using perturbation methods and single and double excitation coupled-cluster theory with noniterative treatment of triple excitations CCSD(T) and the correlation-consistent basis sets supplemented by bond functions placed at the midpoint of the van der Waals bond. Vertical excitation electronic spectra of the diatomic $CO - Ar$ van der Waals molecule will be presented.