

AB INITIO INVESTIGATION OF C_2H_2/X VAN DER WAALS COMPLEXES (X=NOBLE GAS, CO_2 , N_2O).

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We will present ab initio calculations performed at the MP2 and CCSD(T) levels of theory on acetylene containing complexes. We used large basis sets including or not midbond functions and corrected all results for the basis set superposition error. The influence of the monomer geometries on the properties of the complexes has been investigated. The topology of the intermolecular potential energy surfaces of the various complexes will be compared and the methodological approach adapted to the considered systems will be discussed.