AB INITIO TEST STUDY ON THE VERTICAL EXCITATION ENERGY OF VAN DER WAALS DIMERS

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Studies in the framework of the supermolecule approach using high level ab initio methods of quantum chemistry with different basis sets, constructed to give accurate values for the electric moments and polarizabilities, and supplemented by bond functions placed at the midpoint, will be discussed. Vertical excitation electronic spectra of the diatomic van der Waals $CO - H_2$, $CO - He$ and $N_2 - He$ molecules will be presented and compared with recent experimental results.