AB INITIO INVESTIGATIONS ON THE TRIMERS CONTAINING HC_3N IN COMBINATION WITH H_2C_2 AND/OR HCN

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The present contribution focuses on the main results coming from ab initio investigations carried out on the mixed trimers containing (at least one molecule of) cyanoacetylene in combination with acetylene and/or hydrogen cyanide units. The several optimized structures corresponding to true minima on the PES of these complexes have been characterised at different levels of theory, and a set of their spectroscopic parameters relevant to rotational and vibrational spectroscopies have been determined. Besides, by employing different approaches, also the kinds and the topologies of the interactions present in each of these minima have been investigated.