AB INITIO THEORETICAL STUDY OF CARBON CHAINS

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Carbon chains are molecules of great astrophysical interest. We have performed the ab initio study of $C4$, $C5$ and $C6$. We present the structures of the ground state of each molecule as well as the structures of various isomers. These have been calculated using B3LYP and CCSD(T) with cc-pVTZ basis. Besides, we have studied its vertical excitation energies and we propose some of the possible isomerization processes. Finally, we present some spectroscopic parameters, anharmonic constants and the lowest energy levels calculated from the force field determined from the potential energy surfaces around the minima. This calculation are made using MRCI and CASPT2 with cc-pVTZ and ANO-L basis.