SPECTROSCOPY AND STRUCTURE OF CHAINS TYPE C_n, C_nH and C_nSi

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Structures, vertical excitation energies to the first electronic states and spectroscopic parameters for the ground electronic state are determined for several small C_n, C_nH and C_nSi astrophysically important molecular species [a]. The main aim of these investigations is to help the interpretation of several previous astrophysical observations [b] State-of-the art ab initio calculations are performed for this purpose. All species display isomerism although the inter-transformation processes, that involve various electronic states, are not well known. Anharmonic spectroscopic parameters are computed from full-dimensional Potential Energy Surfaces which are mapped close to their respective local minima. In light of these calculated properties (band positions, spectroscopic parameters, predictions of ro-vibronic effects, spin-spin constants,..) assignments for FIR astrophysical observed bands, are discussed. vspace1em

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[b] J. Goicoechea, J. Cernicharo, H. Massó and M.L. Senent, *ApJ.* **609**, 225 (2004); J. Cernicharo, J.R. Goicochea and Y. Benilan, *ApJ* **580**, L157, 2002.