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Resonance Raman study of polyynes inside single-walled carbon nanotubes. MARCOS PIMENTA, LEANDRO MALARD, Departamento de Fisica, Universidade Federal de Minas Gerais, DAISUKE NISHIDE, Department of Chemistry, Nagoya University, ANA PAULA GOMES, ADO JORIO, Departamento de Fisica, Universidade Federal de Minas Gerais, HISANORI SHINOHARA, Department of Chemistry, Nagoya University — We report a resonance Raman study of polyynes CnH2 molecules (n= 10 and 12) composed of linearly bonded sp-carbon atoms aligned inside the single-walled carbon nanotubes (SWNTs), using many laser lines in the range 1.9 to 2.7 eV. The C10H2@SWNT hybrid material exhibits a Raman peak at 2066 cm-1 related with the stretching vibration of the C10H2 molecules interacting with SWNTs, while the C12H2@SWNT exhibits a peak at a lower frequency, around 2020 cm-1. The intensities of these peaks are strongly dependent on the laser energy, and exhibit maxima around 2.15 and 2.10 eV for the C10H2@SWNT and C12H2@SWNT materials, respectively. However, the optical absorption spectrum of the purified C10H2 and C12H2 dispersed in n-hexane exhibits peaks in the UV, around 4.9 and 4.5 eV, respectively.This result can be associated with a two-photon Raman resonance enhancement or can reflect important changes in the electronic structure of the polyynes when they are encaged in a carbon nanotube. New experimental and theoretical works are needed to understand this result.

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