Title:	Heat capacity of endohedral carbon nanotubes Rg@CNT (Rg = He, Ne, Ar and Kr)
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Abstract:	The molar heat capacity of a carbon nanotube encapsulating rare gas atoms He, Ne, Ar and Kr is predicted using the vibrational frequency values computed by ab initio Hartree-Fock method and Density Functional Theoretic method using the M06-2X functional and the 6-31G* basis set. The computed frequency values are compared with the results obtained using an analytical function proposed by Cox et al. (2007). The molar heat capacity results are interpreted in terms of a particle-in-a-cylinder model and a three-dimensional confined harmonic oscillator model.
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