CALCULATED DEPENDENCE OF VIBRATIONAL BAND FREQUENCIES OF SINGLE-WALLED CARBON NANOTUBES ON DIAMETER

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We have used density functional theory (DFT) at the B3LYP/6-31G level to calculate Raman and IR spectra of the fourteen zigzag (n, 0) single-walled carbon nanotubes (SWCNTs) and (n, 0)(2n, 0) double walled carbon nanotube (DWCNTs) that have n ranging from 6 to 19 for SWCNTS, n = 6 to 8 for DWCNTs. In the low frequency RBM region, calculated Raman spectra of SWCNTs indicated that there are three vibrational modes, of symmetries A_1g, E_1g and E_2g, whose frequencies depend strongly on nanotube diameter. The E_2g g mode is not only diameter dependent, but also the even and odd number hexagon formed in the circumference direction of the CNTs. There are also two IR spectral modes (of A2u and E1u symmetries) found in calculated IR spectra with strong diameter dependencies. We have also found three Raman bands with E_1g, A_1g and E_2g symmetries to exist in the G-band region. For this latter case, computed spectra indicated that while Raman bands with A1g symmetry essentially remain constant for the even number hexagon formed in the circumference direction ((0, 2n)-type CNTs; with band position 1526 61617; 0.5 cm^{-1}), but that for (0, 2n+1)-type CNTs are diameter dependent. The frequencies of the E_1g and E_2g modes (in the G-band region) are not only strongly diameter dependent, but also expected to converge towards one another with increasing tube diameter. This latter type of behavior can lead to erroneous classification of nanotubes as metallic or semiconducting, since partially overlapping bands in the G-band region might result in bands with diffuse shoulder, a characteristic of metallic SWCNTs. The RBMs for DWCNTs are also strongly diameter dependent and are blue shifted reference to their corresponding RBMs in the spectra of SWCNTs. The relative distance between RBMs vibrational modes in the spectrum of a desired DWCNT is larger than that for the corresponding SWCNTs. The electron density for the small sized DWCNT, (6,0)(12,0), indicated an intertube CC chemical bonding in the excite state.