Structure-Assigned Emission and Absorption Spectra of Single-Walled Carbon Nanotubes

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The recent discovery of band-gap fluorescence from single-walled carbon nanotubes (SWNT) isolated in aqueous surfactant suspensions opens many new opportunities to basic and applied researchers. In the first major application of SWNT fluorescence, we report a spectrofluorimetric study that reveals distinct electronic transitions for more than thirty different semiconducting nanotube species. Excitation of second van Hove transitions is followed by emission at the corresponding first van Hove near-infrared wavelengths. Through careful pattern analysis of the spectral data, supplemented by a set of resonance Raman measurements, we have assigned each optical transition to a specific (n,m)nanotube structure. Analysis of spectral intensities shows a tube diameter distribution that peaks at 0.93 nm, and a chiral angle distribution that favors near-armchair over zigzag structures. Near-armchair species ranging from (5,4) to (10,9) are detected in our HiPco sample. The observed transition wavelengths deviate significantly from a linear dependence on tube diameter. The dependence of these deviations on chiral angle and tube diameter suggest that a combination of trigonal warping and excitonic effects are present. In addition to giving valuable information on nanotube electronic structures, these findings provide a practical method for rapidly determining the detailed composition of nanotube samples.

References

M. J. O'Connell, et al., *Science* **297**, 593 (2002) S. M. Bachilo, et al., *Science*, in press.