Chapter 8
Cluster Origin of Solvation Features of C-Nanostructures in Organic Solvents

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ABSTRACT

The existence of fullerenes, Single-Wall Carbon Nanocones (SWNCs), especially Nanohorns (SWNHs), Single-Wall Carbon Nanotube (SWNT) (CNT) (NT), NT-Fullerene Bud (NT-BUD), Nanographene (GR) and GR-Fullerene Bud (GR-BUD) in cluster form is discussed in organic solvents. Theories are developed based on columnlet, bundlet and droplet models describing size-distribution functions. The phenomena present a unified explanation in the columnlet model in which free energy of cluster-involved GR comes from its volume, proportional to number of molecules n in cluster. Columnlet model enables describing distribution function of GR stacks by size. From geometrical considerations, columnlet (GR/GR-BUD), bundlet (SWNT/NT-BUD) and droplet (fullerene) models predict dissimilar behaviours. Interaction-energy parameters are derived from C_{60}. An NT-BUD behaviour or further is expected. Solubility decays with temperature result smaller for GR/GR-BUD than SWNT/NT-BUD than C_{60} in agreement with lesser numbers of units in clusters. Discrepancy between experimental data of the heat of solution of fullerenes, CNT/NT-BUDs and GR/GR-BUDs is ascribed to the sharp concentration dependence of the heat of solution. Diffusion coefficient drops with temperature result greater for GR/GR-BUD than SWNT/NT-BUD than C_{60} corresponding to lesser number of units in clusters. Aggregates $(C_{60})_{13}$, SWNT/NT-BUD_7 and GR/GR-BUD_3 are representative of droplet, bundlet and columnlet models.

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INTRODUCTION

Interest in nanoparticles (NPs) arises from the shape-dependent physical properties of materials at the nanoscale (Faraday, 1857; Murphy *et al*., 2010). Occurrence of single-wall carbon nanocones (SWNCs) was used to investigate nucleation and growth of curved C-nanostructures (NSs) suggesting pentagon role. When a pentagon is introduced into a graphitic sheet nanographene (GR) (Figure 1d) *via* extraction of a 60º sector from the sheet one forms a cone leaf. Pentagons presence in an SWNC apex is analogue of their occurrence in single-wall C-nanotube (NT) (CNT) (SWNT) tip topology (*cf*. Figure 1b). Terminations of SWNTs attracted interest once Tamura & Tsukada (1995) theoretically predicted peculiar electronic states related to GR topological defects. Kim *et al*. (1999) observed resonant peaks in density of states (DOS) in SWNTs and Carroll *et al*. (1997), in multiple-wall (MNTs) C-nanotubes (MWNTs).

The SWNCs with discrete opening angles (apices, θ) of 19º, 39º, 60º, 85º and 113º of cone (*cf*. Figure 2) were observed in a C-sample generated by hydrocarbon (HC) pyrolysis (Krishnan *et al*., 1997), which was explained by a cone-wall model composed of wrapped GR sheets where geometrical requirement for seamless connection accounted for semidiscrete character and absolute values of cone angle. Total

Figure 1. Arrangement of C-nanostructures: (a) C_{60}; (b) SWNT; (c) NT-BUD; (d) GR; (e) GR-BUD