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, $\theta$) 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