

Chapter 8

Cluster Origin of Solvation Features of C–Nanostructures in Organic Solvents

Francisco Torrens

Universitat de València, Spain

Gloria Castellano

Universidad Católica de Valencia, Spain

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-BUD₇ and GR/GR-BUD₃ are representative of droplet, bundlet and columnlet models.

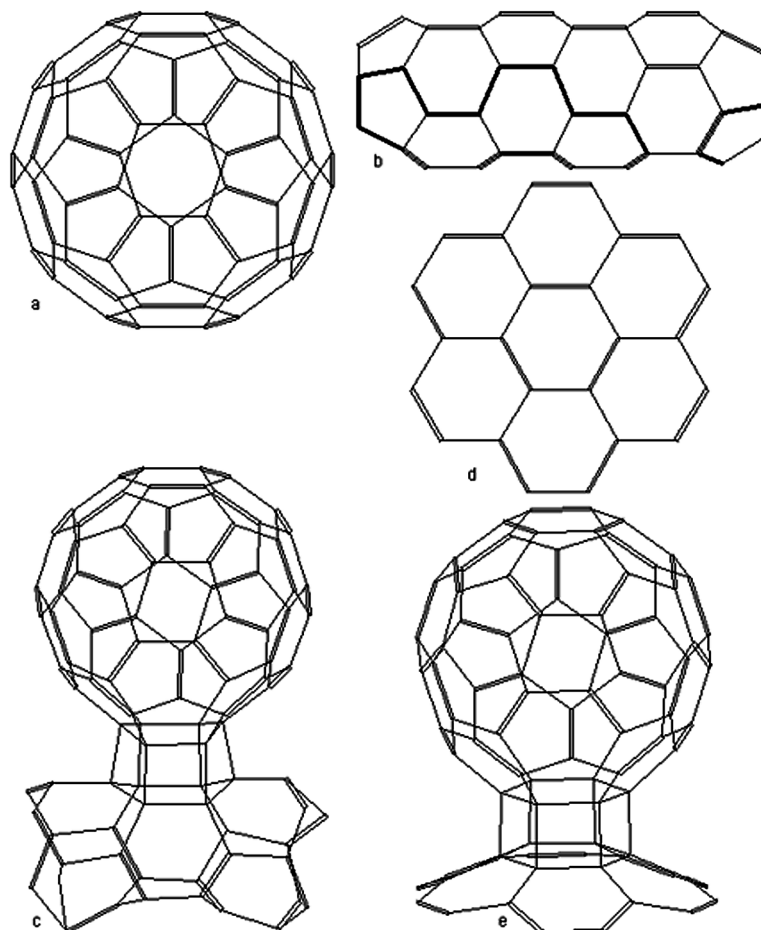
DOI: 10.4018/978-1-5225-0248-7.ch008

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 60° 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 19°, 39°, 60°, 85° and 113° 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



103 more pages are available in the full version of this document, which may be purchased using the "Add to Cart" button on the publisher's webpage:

www.igi-global.com/chapter/cluster-origin-of-solvation-features-of-c-nanostructures-in-organic-solvents/150020

Related Content

QSPR/QSAR Analyses by Means of the CORAL Software: Results, Challenges, Perspectives

Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Orazio Nicolotti, Angelo Carotti, Karel Nesmerak, Aleksandar M. Veselinovi, Jovana B. Veselinovi, Pablo R. Duchowicz, Daniel Bacelo, Eduardo A. Castro, Bakhtiyor F. Rasulev, Danuta Leszczynska and Jerzy Leszczynski (2017). *Pharmaceutical Sciences: Breakthroughs in Research and Practice* (pp. 929-955).

www.irma-international.org/chapter/qsprqsar-analyses-by-means-of-the-coral-software/174156

Marijuana, i.e., Cannabis sativa: The Quandary of Being an Amalgamate of a Useful and Abusive Medicinal Herb

Javid Manzoor, Sajood Ahmad Bhat and Anuradha Sharma (2023). *Cannabis sativa Cultivation, Production, and Applications in Pharmaceuticals and Cosmetics* (pp. 153-171).

www.irma-international.org/chapter/marijuana-ie-cannabis-sativa/320674

Molecular Docking Technique to Understand Enzyme-Ligand Interactions

Kailas Dashrath Sonawane and Maruti Jayram Dhanavade (2017). *Pharmaceutical Sciences: Breakthroughs in Research and Practice* (pp. 727-746).

www.irma-international.org/chapter/molecular-docking-technique-to-understand-enzyme-ligand-interactions/174148

Application of Nanoparticles as a Drug Delivery System

Vijay Kumar Singha and Raj K. Keservani (2017). *Novel Approaches for Drug Delivery* (pp. 364-389).

www.irma-international.org/chapter/application-of-nanoparticles-as-a-drug-delivery-system/159673

Ethnobotanical, Pharmacological, and Therapeutic Importance of Basil Seeds Along With Their Role in the Biogenic Synthesis of Important Chemical Substances

Hafsa Javaid, Mahrukh Khan, Mehrab Khan, Javeria Kanwal and Maryam Asghar (2024). *Therapeutic and Pharmacological Applications of Ethnobotany* (pp. 38-73).

www.irma-international.org/chapter/ethnobotanical-pharmacological-and-therapeutic-importance-of-basil-seeds-along-with-their-role-in-the-biogenic-synthesis-of-important-chemical-substances/344956