

**TITLE**

**Cluster bundlet model of single-wall C, BC<sub>2</sub>N and BN nanotubes, nanocones and nanohorns**

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It is discussed the existence of single-wall carbon nanocones (SWNCs) especially nanohorns (SWNHs), and their BC<sub>2</sub>N and boron nitride (BN) analogues in organic solvents in the form of clusters. A theory is developed based on a bundlet model describing their distribution function by size. The phenomena present a unified explanation in the bundlet model in which the free energy of an (BC<sub>2</sub>N/BN-) SWNC, involved in a cluster, is combined from two components: a volume one proportional to the number of molecules  $n$  in a cluster and a surface one proportional to  $n^{1/2}$ . The bundlet model enables describing the distribution function of (BC<sub>2</sub>N/BN-) SWNC clusters by size. From purely geometrical differences the bundlet [(BC<sub>2</sub>N/BN-) SWNCs] and droplet (C<sub>60</sub>/B<sub>15</sub>C<sub>30</sub>N<sub>15</sub>/B<sub>30</sub>N<sub>30</sub>) models predict different behaviours. The (BC<sub>2</sub>N/BN) SWNCs of various disclinations are investigated via energetic and structural analyses. Several (BC<sub>2</sub>N/BN) SWNC's terminations are studied, which are different among one another because of the type of closing structure and arrangement. The packing efficiencies and interaction-energy parameters of (BC<sub>2</sub>N/BN) SWNCs/SWNHs are intermediate between those of C<sub>60</sub>/B<sub>15</sub>C<sub>30</sub>N<sub>15</sub>/B<sub>30</sub>N<sub>30</sub> and (BC<sub>2</sub>N/BN) single-wall carbon nanotube (SWNT) clusters: an in between behaviour is expected; however, the properties of (BC<sub>2</sub>N/BN) SWNCs especially (BC<sub>2</sub>N/BN) SWNHs are calculated closer to (BC<sub>2</sub>N/BN) SWNTs. The structural asymmetry in the different (BC<sub>2</sub>N/BN) SWNCs, entirely characterized by cone angle, distinguishes the properties of some ones. The heat of solution varies:  $P2 \approx P1 > P3 > P4 > \text{SWNH} \approx \text{SWNT} \gg \text{C60}$ . It seems that BC<sub>2</sub>N/BN will be stable especially those species isoelectronic with C-analogues.

**Biography**

Francisco Torrens is BSc, Universitat de València, 1984, MSc, 1987, PhD, 1990, PhD talent prize, 1991, PhD grant, 1987-91, 74 congress organizations, editor-in-chief of Meeting in Science, Technology, Education and Gender, editor of Molecules, MATCH Communications in Mathematical and in Computer Chemistry, Research Journal of BioTechnology, Research & Reviews in BioSciences, Asian Journal of Biochemistry, Asian Journal of Scientific Research, Biotechnology, International Journal of Biological Chemistry, Current Drug Discovery Technologies, Journal of WSCG, African Journal of Biochemistry Research, Molecular Diversity, African Journal of Pure and Applied Chemistry, African Journal of Pharmacy and Pharmacology, International Journal of Liquid State Sciences, etc.