It is discussed the existence of single-wall carbon nanocones (SWNCs), especially nanohorns (SWNHs), in organic solvents in the form of clusters [1]. A theory is developed based on a *bundlet* model, describing their distribution function by size [2]. The phenomena have a unified explanation in the bundlet model, in which the free energy of an 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 \( n^{1/2} \) [3]. The bundlet model enables describing the distribution function of SWNC clusters by size. From purely geometrical differences the bundlet (SWNCs) and droplet (fullerene) models predict different behaviours. The SWNCs of various disclinations are investigated via energetic-structural analyses (*cf.* Fig. 1). Several SWNC's terminations are studied, which are different among one another because of the type of closing structure and arrangement (*cf.* Fig. 2). The packing efficiencies and interaction-energy parameters of SWNCs/SWNHs are intermediate between the ones of fullerene and single-wall carbon nanotube (SWNT) clusters; an in-between behaviour is expected. However, the properties of SWNCs, especially SWNHs, are calculated close to SWNTs. The structural asymmetry in the different SWNCs, entirely characterized by their cone angle, distinguishes the properties of some ones: P2, etc. Provisional conclusions follow. (1) Close packings are the tightest way to pack spheres: atoms and fullerenes being nothing but tiny spheres often arrange in this way. Furthermore, it is possible to deduce atomic structures of metal alloys, salts and oxides by fitting the voids of close-packed spheres. Several criteria were selected to reduce the analysis to a manageable quantity of packing properties and objects, from the enormous set of equal things. The former refer to three properties: packing closeness, dimension and efficiency. A model could reliably predict a packing entity's property, if article is sufficiently similar in structure to the group of items used to generate the model. The two-step approach, involving object clustering and property prediction, provided an efficient way to assess the reliability of a model's prediction. The non-computationally intensive approach not only solved the problem, but also has practical applications in modelling. (2) The packing efficiencies and interaction-energy parameters of nanocones are intermediate between the ones of fullerene and single-wall carbon nanotube clusters. Therefore an in-between behaviour was expected. However, the packing efficiencies and interaction-energy parameters of nanocones are close to the ones of nanotube clusters. As a result a nanotube-like behaviour is observed as expected, and the properties of nanocones are calculated closer to the ones of nanotubes and more distant from the ones of fullerene. (3) The packing efficiency and interaction-energy parameters of nanohorns are the closest to the ones of nanotube clusters. The most nanotube-like behaviour is observed, and the properties of nanohorns are calculated the closest to the ones of nanotubes. (4) The large structural asymmetry in the different types of nanocones, entirely characterized by their number of pentagons in one–five, allows distinguishing the calculated properties of some kinds especially the cone with two pentagons. Work is in progress on the possible generalization of the conclusions above to more complex systems, *e.g.*, single-wall boron nitride (BN) nanocones.
References


Figures

Figure 1. $C_{60}$–SWNT–SWNC interaction energy with its surroundings in cluster volume or surface.

Figure 2. Temperature dependence of solubility of $C_{60}$ (droplet)–SWNT/SWNC (bundlet).