Model Narrow Nanotubes Related to C_{36}, C_{32} and C_{20}: Computational Structural Sampling

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Very recently, narrow nanotubes have been observed with a diameter of 5 Å (Sun *et al.*, Nature **403** (2000) 384) and even with a diameter of 4 Å (Qin *et al.*, Nature **408** (2000) 50). It has been supposed that the narrow nanotubes are closed by fragments of C_{36} and C_{20} fullerenes. The contribution reports computations on related model nanotubes with stoichiometries like C_{84}, C_{96} or C_{80}. Computations are carried out at the PM3, SAM1, and B3LYP/6-31G* levels. Two C_{36} fullerenes are considered, D_{6h} and D_{2d}, and, for example, at the PM3 level and with the C_{84} nanotube stoichiometry the D_{2d} cage closure gives a lower energy (by 185 kcal/mol and diameter of 5.42 Å). There is another possible candidate, C_{32} cage with a D_{4d} symmetry. At the PM3 level and with the C_{96} nanotube stoichiometry the D_{4d} closure has the nanotube energy lower by 210 kcal/mol (with the nanotube diameter of 5.43 Å) compared to the D_{6h} nanotube closure. On the other hand, four-membered rings should not play a significant role in the narrow nanotubes with the diameter of 4 Å, where the dodecahedron-related closure should be exclusive. The findings are also supported by the B3LYP/6-31G* calculations.