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Topology counting in nanostructures

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ABSTRACT. Tubulenes are capped nanotubes built up from two caps and a distancing nanotube/neck of diverse decoration. Ways of "in silico" construction of several finite nanostructures, classified by their neck and/or caps, are presented. Topological periodicity is presented as constitutive typing enumeration. Semiempirical calculations support the idea that new, relatively stable molecules may appear in the soot of vaporized graphite.

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