Thermodynamics and Kinetics of Oxygen Addition to Model Nanotubes: A Computational Study

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It has been known for fullerenes that the computed thermodynamic and kinetic terms give different picture for oxygen additions to selected bonds. In fact, only the computed kinetic stability order agrees with what is known from observations. It has been suggested that the oxygen addition to fullerenes is kinetically rather than thermodynamically controlled. A similar question can be asked for nanotubes as their oxidation has also been known. In contrast to fullerenes, however, in computations only some simplified models of nanotubes can be studied by quantum-chemical methods as computational demands increase rapidly with the number of atoms. Thus, narrow nanotubes observed recently are particularly convenient for the computations. Moreover, they should also be more reactive. In this report we perform calculations of oxygen additions to such model nanotubes capped by fragments of D_{2d} and D_{6h} C_{36} fullerene cages or by a fragment of C_{32} *quasi*-fullerene cage with two four-membered rings, or finally by a fragment of dodecahedral C_{20}. Both thermodynamic enthalpy changes and kinetic activation barriers for oxygen addition to selected bonds are computed and analyzed.