Enhanced Permeability of Fluorinated Carbon Nanocages for Medicine
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Carbon nanocages (buckyball $C_{60}$ or larger fullerenes and nanotubes) could be convenient shells-carriers for radioactive isotopes and other components for a variety of medical applications (treatment, image-contrast, diagnostics, etc.). However, their utility is principally hindered by the difficulties of incorporation of most of the elemental components: the yield of the desired structures $X@C$ is extremely low. This is due to large activation barriers for penetration inside the cages and is often complicated by the binding of the ions to the $\pi$-electrons.

Theoretical analysis indicates that such barriers can be reduced if the $\pi$-subsystem of electrons is depleted by the covalently attached fluorine (e.g. in a $C_{60}F_{48}$ as shown in the Fig. 1). We have performed preliminary calculations and evaluation of the potential barrier reduction, which appears to be substantial. For example, calculations show that while the hexagon-center entry of a proton $H^+$ has a barrier near 6 eV, the similar trajectory barrier for the fluorinated cage is three times lower, near 2 eV. In fact, approximately the same barrier reduction is attained for the “holes” near the hexagon centers of about 1.5 Å size, equivalent to nearly 25% of the cage “surface area”.

This suggests that the yield of the endohedral units $X@CF$ must be much higher than that of non-fluorinated $X@C$. It opens new ways for the efficient synthesis of useful endohedral components by either ion beam irradiation or high-pressure/temperature processing [see for example (1)], following the stage of fluorination that can be achieved by previously described methods (2). Detailed quantum-chemical computations (3) must lead to a more accurate assessment of the yield and required conditions for a series of interesting compositions like $X@CF$ ($X=H$, $T$, $H_2$, $Li$, $Co$ etc.)

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REFERENCES