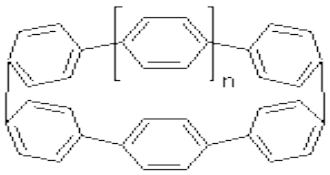
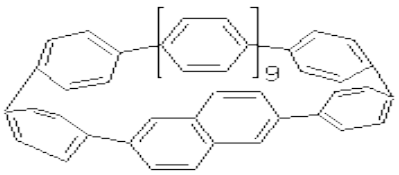
CHIRAL NANOHOOPS

Single-walled carbon nanotubes (SWNT) can be thought of as built from component macrocycles, often called nanohoops. So, for example, cycloparaphenylenes like **1** can be the thought of as the precursor (at least in principle) of armchair SWNTs. To create chiral SWNTs, Itami[1] has suggested that cycloparaphenylene-naphthalene (**2**) and other acene substituted macrocycles would serve as appropriate precursors.



1

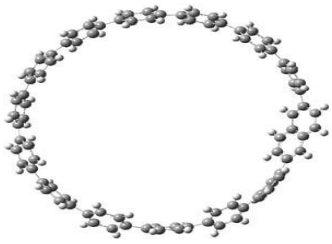


2

Itami has synthesized **2** (having 13 phenyl groups and one naphthyl group) and also examined the ring strain energy and racemization energy of a series of these types of compounds at B3LYP/6-31G(d). As might be expected, based on studies of the cycloparaphenylenes themselves,[2,3] ring strain energy decreases with increasing size of the macrocycle. So, for example, the macrocycle with one naphthyl group and 5 phenyl rings has a strain energy of 90 kcal mol^{-1}, but the strain is reduced to 40 kcal mol^{-1} with 13 phenyl rings.

The macrocycle **2** and related structures are chiral, existing in *P* and *M* forms. The racemization involves first rotation of the naphthyl group, as shown in Figure 1, with a barrier of about 8 kcal mol^{-1}. The direct product has the opposite stereochemistry but is not in the lowest energy conformation. Rotations of some phenyl groups remains to occur, but these rotations are expected to have a barrier less than that for the rotation of the naphthyl group, based on the previous study of cycloparaphenylenes. Again, the racemization barrier decreases with the size of the macrocycle.

(*P*)-**2** **2-TS**



(*M*)-**2'**

Figure 1. B3LYP/6-31G(d) optimized structures along the racemization pathway of **2**.
Source: http://comporgchem.com/blog/?p=1561