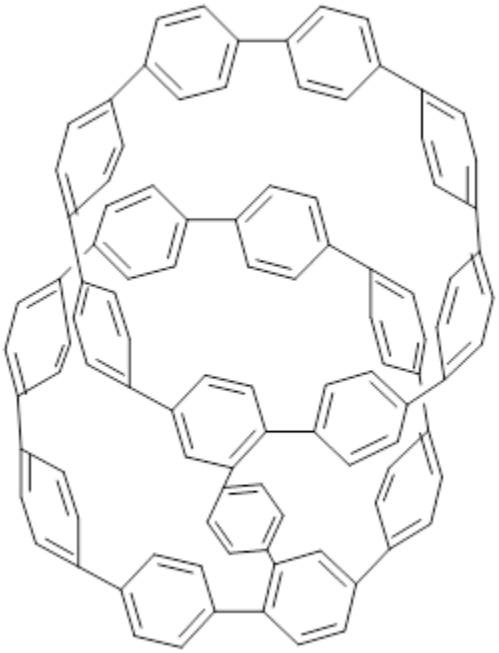
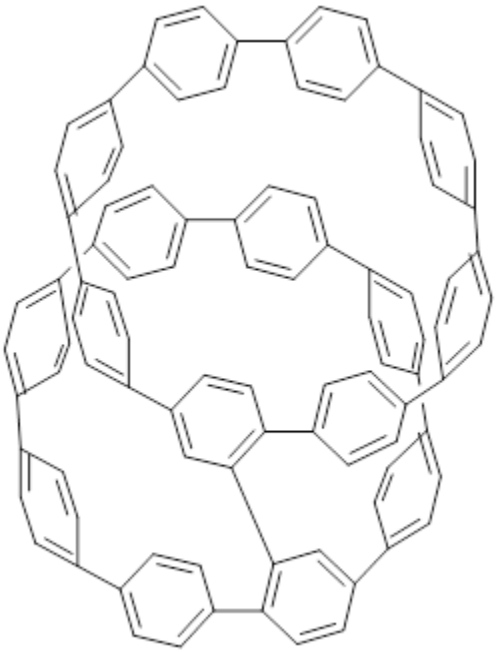
COVALENTLY LINKED CYCLOPARAPHENYLENES – ONWARDS TO NANOTUBES

Nanotubes are currently constructed in ways that offer little control of their size and chirality. The recent synthesis of cycloparaphenylenes (CPP) provides some hope that fully controlled synthesis of nanotubes might be possible in the near future. Jasti has now made an important step forward in preparing dimers of CPP such as **1**.[1]

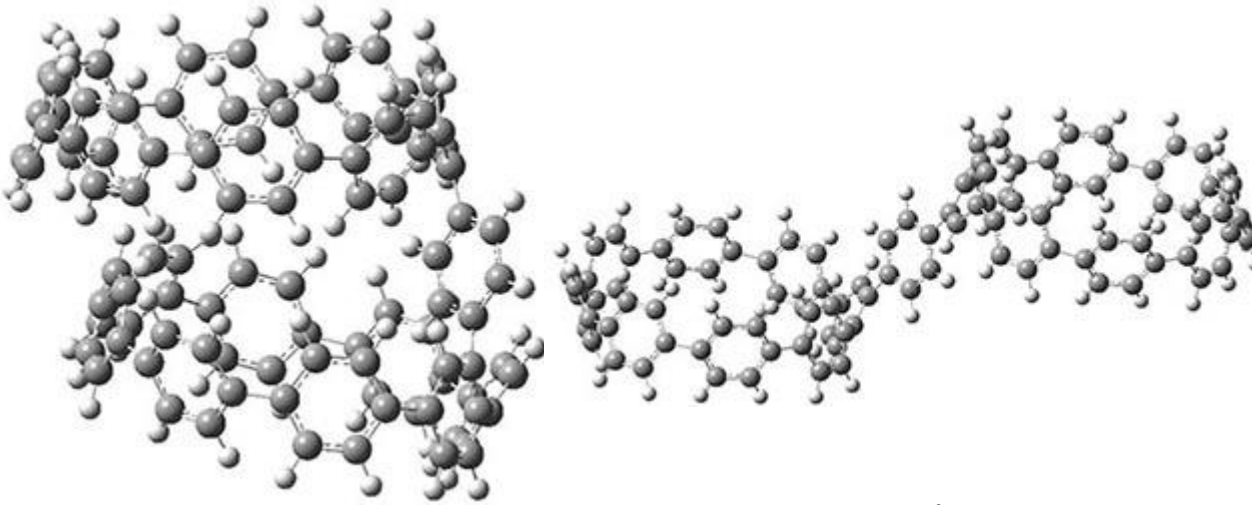


1



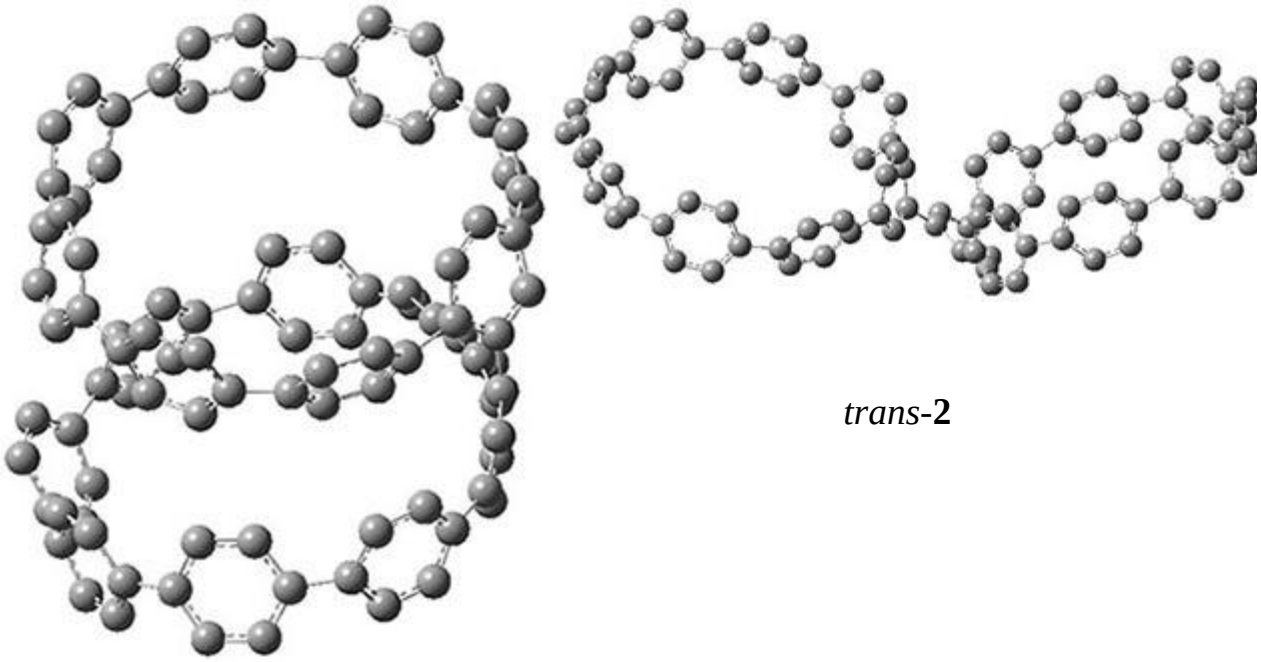
2

They also performed B3LYP-D/6-31G(d,p) computations on **1** and the directly linked dimer **2**. The optimized geometries of these two compounds in their *cis* and *trans* conformations are shown in Figure 1. Interestingly, both compounds prefer to be in the *cis* conformation; *cis*-**1** is 10 kcal mol^{-1}more stable than *trans*-**1** and *cis*-**2** is 30 kcal mol^{-1} more stable than the *trans* isomer. While a true transition state interconnecting the two isomers was not located, a series of constrained optimizations to map out a reaction surface suggests that the barrier for **1** is about 13 kcal mol^{-1}. The authors supply an interesting movie of this pseudo-reaction path.



trans-**1**

cis-**1**



trans-**2**

cis-**2**

Figure 1. B3LYP-D/6-31G(d,p) optimized geometries of the *cis* and *trans* conformers of **1** and **2**.

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