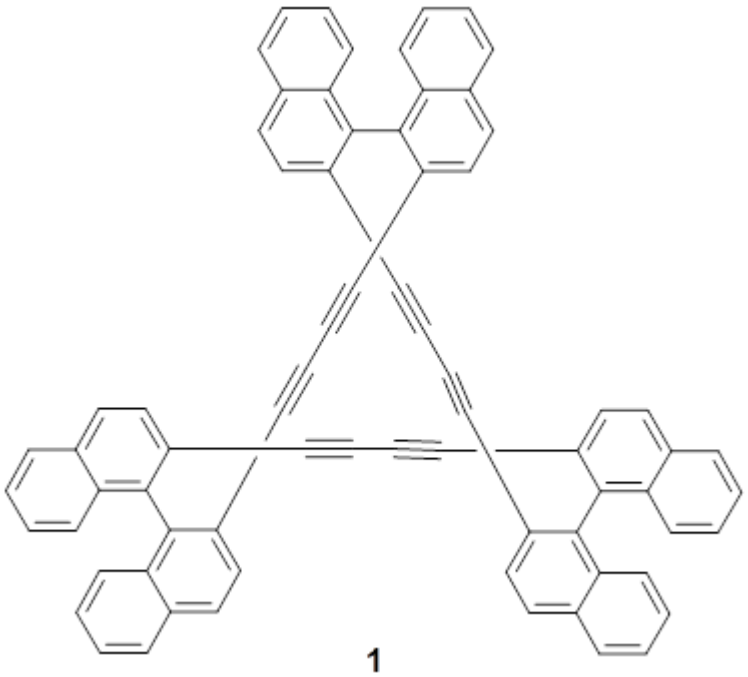
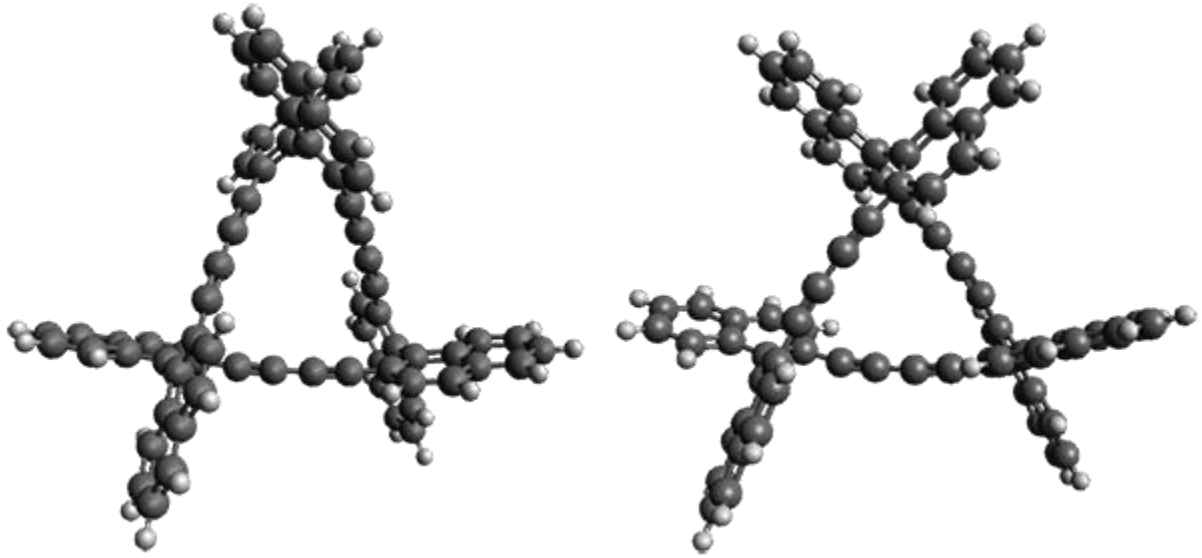
DESIGN AND SYNTHESIS OF THE FIRST TRIPLY TWISTED MÖBIUS ANNULENE

Herges and co-workers have prepared a triply-twisted Möbius molecule. [1] The key element is recognizing that most of the "twisting" needs to be accomplished through *writhe*, a twisting that produces figure-8-like crossing, the way an old-school phone cord twists about itself or the way a pretzel is formed. Herges employs three bi-naphthelene subunits to provide the template for the writhe needed. The prepared compound is **1**. A clever, relatively straightforward synthesis produces this amazing molecule, along with the single-twisted **2**.



1

The B3LYP/6-31G* optimized geometries of **1** and the single-twisted analogue **2** are shown in Figure 1. Table 1 presents the key topological parameters of **1** and **2**, comparing the computed and X-ray crystal structure. The absolute value of the linking number L_k is 3, indicating the three twists, and the reason that this highly twisted molecule can be made is that half of the twist actually results from writhe.



1 **2**

Figure 1. B3LYP/6-31G* optimized geometries of the two diastereomers if **1**. (Be sure to click on these images to launch JMol and interactively manipulate the structures!)

Table 1. Topological parameters of **1**. [a]

	$\|L_k\|$	$\|T_w\|$	$\|W_r\|$
X-ray, **1**	3.0	1.42	1.58
Comp, **1**	3.0	1.33	1.67
Comp, **2**	1.0	0.37	0.63

[a] L_k is the linking number, T_w is the twist number, and W_r is the writhe number, with the condition that $T_k + W_r = L_k$.

Source: http://www.compchemhighlights.org/2014/10/design-and-synthesis-of-first-triply.html