2 Summary

For a long time synthetic cyclopeptides, which are based on their natural counterparts, were used for the design of unidirectionally switches. They are also used in the synthesis of host molecules that can bind small molecules, ions or gases.

In the first part of this work, new switching systems were sought, which can be switched in different ways. For this purpose, on the one hand light-inducible systems, like azobenzene (**1**) and different spiropyranes (for example **2**) have been examined. On the other hand redox-inducible molecules, based on a biphenol structure (for example **3** and **4**), were prepared and analyzed via UV spectroscopy (Figure 2.1). The UV spectra of the various switching processes were measured in different solvents to identify the most potent system. An unidirectional switch can be established by connecting the switching unit with a cyclopeptide. Additional cyclic voltammograms of the systems were recorded to determine the redox potentials.

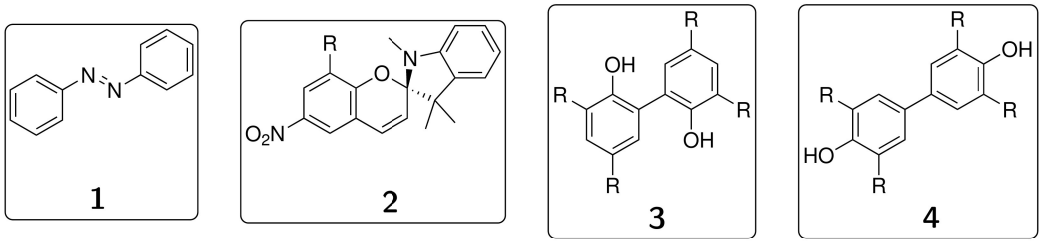

Figure 2.1: Switching systems which were examined in this work.

Also, a combination of these two switching systems (**5**, Figure 2.2) could be synthesized. This double switch can assume four states in series by switching both systems orthogonally. This switching cycle has also been observed in the cyclic voltammogram as well as in the UV spectrum.

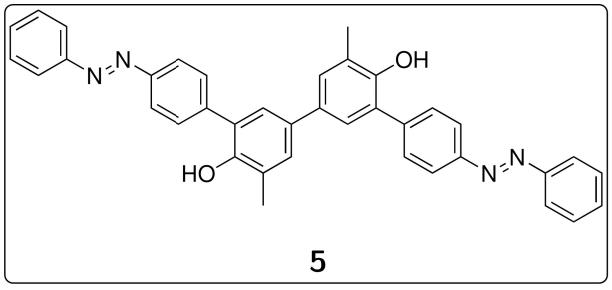

Figure 2.2: Double switch containing two azobenzenes and one 4,4'-biphenole unit.

In the second part of this work, *van-der-Waals* complexes were examined. On the one hand the triphenylphosphine oxide container **6** based on a cyclopeptide scaffold (Figure 2.3) was used. Among other things, unexpectedly high binding constants of the chloroform complex were determined. These were confirmed by dispersion-corrected DFT calculations and DF-DFT-SAPT analysis.

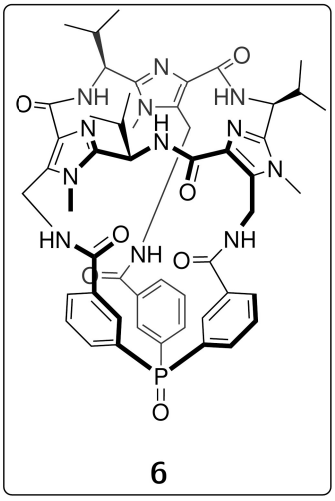

Figure 2.3: The triphenylphosphine oxide container which was examined in this work.

On the other hand, long known cryptophanes (**7** in Figure 2.4) were synthesized and studied in different NMR solvents. So far, relatively small binding constants of the complex chloroform@cryptophane-E (Figure 2.4 (right)) were measured by NMR spectroscopy in deuterated tetrachloroethane. Based on the very high binding constants measured for the complex $CHCl_3$@**6**, it was shown that tetrachloroethane – contrary to scientific consensus – is bound by cryptophane-E (**9**). The binding constants measured to date merely show an equilibrium between the complexes with the solvent respectively chloroform. The values determined in this study are consistent with the energies obtained by dispersion-corrected DFT calculations.

While trying to get a completely empty container, it turned out that an imploded form of cryptophane-E (*impl*; right in Figure 2.5) is stable, not the spherical form (*out-out*; left in Figure 2.5).

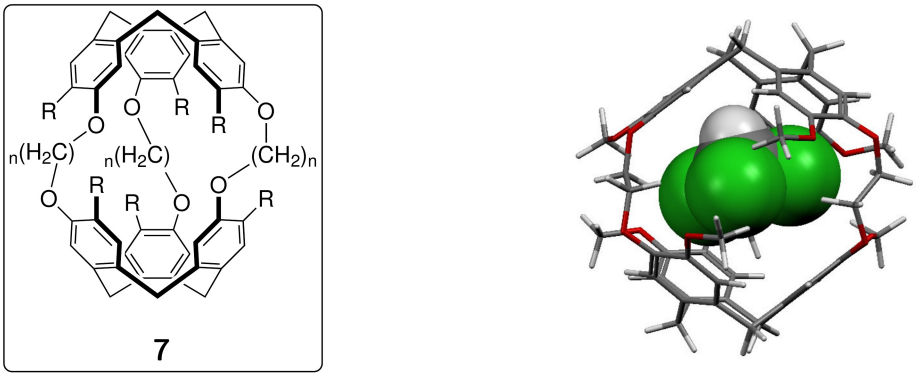

Figure 2.4: General structure of cryptophanes (left) and the complex chloroform@cryptophane-E with $n = 3$ (right).

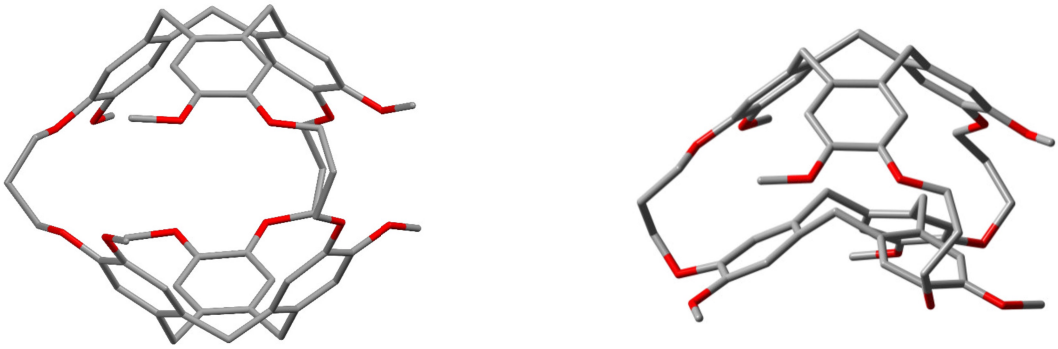

Figure 2.5: Cryptophane-E (**129**) as *out-out-* (left) and as *impl*-form (right).