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Assessment of the PhD Thesis of Ing. Aneta Závodná

“Synthesis of Rotaxane Structures with Multitopic Ligands”

The dissertation of Aneta Závodná discusses innovative approaches toward the synthesis of rotaxanes and studies ways to stimulate the disassembly of these mechanically-interlocked supramolecular structures. For this purpose several multitopic ligand systems were designed and synthetically prepared by the candidate. The implication of these ligands in the formation of rotaxanes with cucurbiturils and therefrom resulting higher-order supramolecular structures was studied under variable conditions by NMR spectroscopy and also isothermal titration calorimetry (ITC). The results of these studies led to a rather complete and deep understanding of the physical organic chemistry of the investigated systems. The perhaps most intriguing result of the work is related to the chemically-induced disassembly of a

cucurbit[6]uril-containing rotaxane by means of the complexation of a cucurbit[7]uril macrocycle at one of the stopper units of a ligand. This opens new avenues for the release of macrocyclic components ready to complex alternative cargo and has been demonstrated beautifully in the present thesis. Noteworthy, this result was also the centerpiece of a recent publication in a top-rated multidisciplinary chemistry journal (*Chem. Sci.* **2025**, *16*, 83–89), that features Aneta Závodná as first author.

In my opinion, the amount of work and countable results, their contextualization as well as their significance for the field of supramolecular chemistry in general and rotaxane chemistry in particular, are very much in accordance with the level of demand on a Ph.D. thesis in chemistry. A high level of rigorous analytical characterization of the synthesized compounds and supramolecular structures (including X-ray crystal structures of rotaxanes!) is recognizable. This expertise is paired with in-depth experiments (NMR titrations, ITC, mass spectrometry, kinetic studies, studies of activation energies, etc.) that allow shining light on various aspects of rotaxane formation and the involved host-guest complexation processes. It is notable that the candidate had to master all these facets and she did so in a highly competent manner.

Beside this main body of results that constitute the resented Ph.D. thesis, the candidate was also involved in several other projects that deal with the host-guest complexation by cucurbiturils. These collaborative efforts within the research group led to another publication in a very well recognized journal (*J. Org. Chem.* **2023**, *88*, 15615–15626).

The thesis work has been developed in a field that is internationally highly competitive and it is certainly not easy to identify innovative study subjects with the potential to add relevant results to the field of rotaxane chemistry. After reading the thesis and also the therefrom

derived publication in *Chemical Science* I am convinced that Aneta Závodná has succeeded in reaching the ambitious proposed objectives. It is not difficult to predict that she has grown as an independently working scientist during the course of the work, receiving formation on all the above mentioned experimental aspects and methodologies that were used. The choice of methods is adequate and the obtained results validate the initial hypotheses.

In my opinion the quality of the dissertation is ranked above average and the obtained results will very likely have a long-lasting impact on the fields of rotaxane chemistry and cucurbituril chemistry. For all abovementioned reasons I recommend the thesis for defense in its present form.

(Uwe Pischel)