ROTAXANES: MOLECULAR MOTION IN THE GAS PHASE

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Rotaxanes, molecules in which the components are mechanically linked but not connected by covalent bonds, are proving useful structural prototypes for helping realize the concept of artificial molecular machinery. We are particularly interested in amide-based rotaxanes in which the hydrogen bonding interactions between the interlocked parts can be modulated, thereby influencing the equilibrium between the various possible co-conformers. The ability to change the relative orientation and position of the macrocycle with respect to the thread is the ultimate key to achieve the desired applications. The first step to induce molecular motions is to affect the hydrogen bond interactions between the macrocycle and the thread.

To be able to control and to manipulate the mechanical motion between the interlocked parts, a proper understanding at the molecular level is required. Therefore, a detailed understanding of the interactions between the macrocycle and the thread in rotaxanes under isolated conditions is obtained by IR-UV double resonance spectroscopy. The use of IR-double resonance spectroscopy is advantageous because the ground state IR spectra directly reveal the hydrogen-bond interactions, since the frequencies of the Amide I and II (C=O stretch and NH bend, respectively) shift significantly when they are involved in hydrogen bonding. Studies of mechanically interlocked molecules and their separate components thus allow us to elucidate the intercomponent interactions.

Here we demonstrate that we can address these interactions and controllably unlock a macrocycle from a thread by adding solvent molecules to a single [2]-rotaxane one at a time. As a result, we are now able to liberate the macrocycle from the thread in a prototypical rotaxane, and are working towards translating this macrocycle along the thread.