MECHANICALLY INTERLOCKED MOLECULES IN THE GAS PHASE: ISOLATED MOLECULE SPECTROSCOPY AND DYNAMICS

W. J. BUMA, A. M. RIJS, *University of Amsterdam, Faculty of Science, Van 't Hoff Institute for Molecular Sciences, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands*; M. S. de VRIES, *University of California Santa Barbara, Department of Chemistry and Biochemistry, Santa Barbara, California 93106, USA*; and D. A. LEIGH, *University of Edinburgh, School of Chemistry, The King's Building, West Mains Road, Edinburgh EH9 3JJ, UK*.

Rotaxanes are compounds that consist of multiple components that are non-covalently bonded. In our case, the rotaxanes consist of one macrocycle which is locked onto the linear thread by hydrogen bonds and trapped by two bulky stoppers. This class of molecules is of particular interest for the development of "molecular motors" since it provides components which can move with respect to each other without falling apart.

We employed laser desorption in combination with supersonic expansions to obtain isolated molecules to study these molecular motors in the gas phase. To fully investigate the structural and spectroscopic properties of these molecular systems a combination of high-resolution spectroscopic techniques have been used, REMPI to obtain the mass-selected vibrational resolved excitation spectra, UV-UV hole-burning to identify the different conformers and IR Ion-Dip spectroscopy to characterize these conformers.

Recent experiments prove that it is possible to seed these supramolecular systems with molecular weight above 1,000 intact into a supersonic beam expansion by using laser desorption. Vibrationally resolved excitation spectra are obtained for the succinic-thread and succinic-rotaxane. IR-UV Ion dip spectroscopy measurements are performed to investigate the N-H and C-H stretch vibrations. The N-H vibrations are highly diagnostic to explore the hydrogen-bonded conformational landscape, i.e. they are used to probe the conformational arrangement of the hydrogen-bonded interlocked components of the studied rotaxane.