Exploring Conductance Phenomena in Single Molecule Break Junctions using Thiophene Macrocycles with Multiple Pathways

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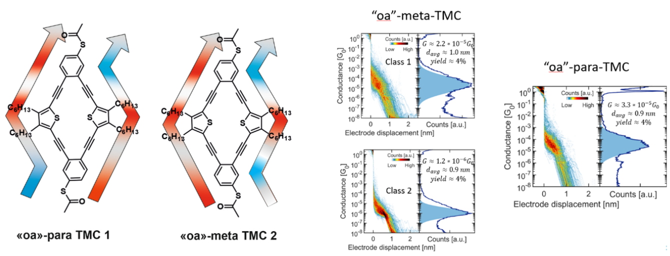
Molecular electronics including the measurement of molecules in single molecule break junctions (SMBJ) is an expanding field of research that leads to an increasing number of new findings[1][2][3]. Recently, the idea of a molecular wire that splits up into two pathways that are equivalent in length sparked our interest since we are interested in interference and phase shift phenomena. For the design of such a system, molecular orbital theory[4], the length of the molecular wire[5], substitutions on connecting units[6] and the kind of anchoring groups[7] must be taken into consideration. Macrocycles **1** and **2** (figure 1 a.) with acetylated thiol anchoring groups were therefore synthesized. These planar, strained, conjugated systems are accessible *via* a series of Sonogashira cross couplings and acetylene deprotections. Following the established substitution rules[4] for good (*para,* figure 1 in red) and poorly conducting (*meta*, figure 1 in blue) electron transport predictions about the overall conductance can be made by adding up the sequential substitution patterns of the connecting corner units. First measurements of both macrocycles **1** and **2** have been performed using the Mechanically Controlled Break-Junction technique. Interestingly, conductance measurements on the “oa”-*meta* TMC show two molecular features, possibly indicating two different pathways for conductance, whilst the “oa”-*para* TMC showed only one in comparison as can be seen in Fig. 1b), c). Further investigations on these systems are ongoing.



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