A Lateral Expansion Strategy for Molecular Spoked Wheels

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A lateral expansion strategy of molecular spoked wheels (MSWs) based on an *all*-phenylene backbone is a task that turned out to be challenging. The MSWs contain a central hub, six spokes and a rim that is formed by a six-fold *Yamamoto* coupling of the respective non-cyclized dodecabromo precursor. Attempts to prepare such compounds without flexible side groups at the spokes were unsuccessful, most probably due to an aggregation and accompanying oligomerization of the precursors during the cyclization. To overcome these problems, fluorene units are introduced at the spokes. These contain additional alkyl chains and lead to a curvature of the wheels. Quantum-chemical calculations using a geometric model and strain calculations predict their synthetic accessibility and subsequently these structures were synthesized with four and even six phenylene units at each edge of the hexagonal wheel. The resulting MSWs were characterized by spectroscopic methods and additionally some of them are visualized via scanning tunneling microscopy (STM).

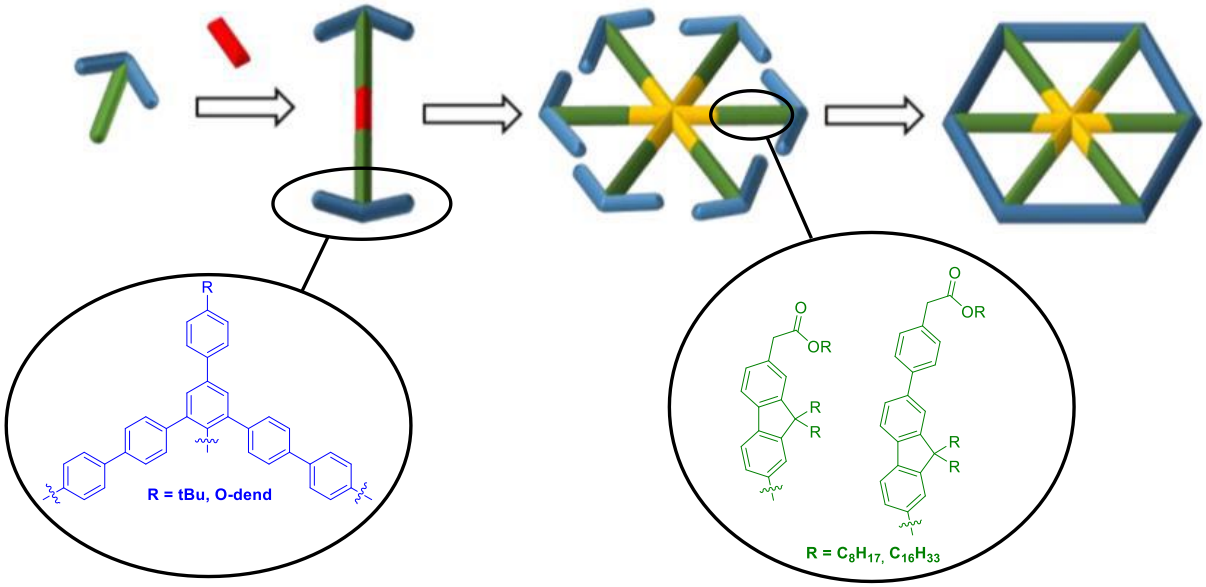

Figure 1: Schematic overview over the synthesis and enlargement of MSWs highlighting some of the key structural motifs.