

Publication

2,5-Diaryl 6-hydroxyphenalenones for Single-Molecule Junctions

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A modular access to 2,5-diaryl 6-hydroxyphenalenone derivatives is developed and demonstrated by a small series of 5 molecules. Within this series, the structures 1 and 2 expose terminal methylsulfanyl anchor groups, enabling their integration in a single-molecule junction. The modular synthesis is based on Suzuki cross-coupling of the aryl substituents as boronic acid precursors with 5,8-dibromo-2-(tert-butyl)-4,9-dimethoxy-2,3-dihydro-1H-phenalen-1-one, and the subsequent transformation of the product to the desired 2,5-diaryl 6-hydroxyphenalenone in a reduction/deprotection sequence. The new structures are fully characterized and their optical and electrochemical properties are analysed. For the derivatives 1 and 2 suitable for single-molecule junctions, the corresponding oxophenalenoxyl radicals 1R and 2R were obtained by oxidation and analysed by electron paramagnetic resonance spectroscopy. Preliminary mechanical break junction experiments with 1 display the structure's ability to form transient single-molecule junctions. The intention behind the molecular design is to profit from the various redox states of the structure (including the neutral radical) as a molecular switch in an electrochemically triggered single-molecule transport experiment.

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