Geländer Molecules with Orthogonal Joints: Synthesis of Macrocyclic Dimers

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Orthogonal joints, understood as connections with an angle of 90ř, were introduced in the design of the "Geländer" model compounds 1 and 2. The banister, consisting of a conjugated carbazole dimer linked by either 1,3-butadiyne (2) or a single thiophene (1), wraps around an axis composed of a phthalimide dimer due to the dimensional mismatch of both subunits, which are interconnected by phenylene rungs. The "Geländer" structure was assembled from a monomer comprising the 1,4-diaminobenzene rung with one amino substituent as part of a 4-bromo phthalimide subunit forming the orthogonal junction to the axis, and the other as part of a masked 2-ethynyl carbazole as orthogonal joint to the banister. The macrocycle was obtained by two sequential homocoupling steps. A first dimerization by a reductive homocoupling assembled the axis, while an oxidative acetylene coupling served as ring-closing reaction. The formed butadiyne was further derivatized to a thiophene, rendering all carbons of the model compound sp2 hybridized. Both helical structures were fully characterized and chirally resolved. Assignment of the enantiomers was achieved by simulation of chiroptical properties and enantiopure synthesis.
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