Unraveling the twist: designing Möbius strip molecules

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[n]Möbiusenes, circlets of catacondensed aromatic rings with a half twist, are severely strained as a result of the confluence of geometrical and topological constraints. We have derived a mathematical model of these constraints. Less severely strained analogs of these chiral structures have been designed, based on the mathematical model. Structures of the analogs were computed using molecular mechanics, AM1 and HF/3-21G.