

A Combined Experimental and Theoretical Study on the Stereodynamics of Monoaza[5]helicenes: Solvent-Induced Increase of the Enantiomerization Barrier in 1-Aza-[5]helicene

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Helicenes and heterohelicenes are attractive compounds with great potential in materials sciences to be used in optoelectronics as ligand backbones in enantioselective catalysis and as chiral sensors.[1] Synthetic protocols were developed to obtain helicenes with skeletons consisting of ortho-fused benzene rings or analogue structures incorporating a heteroatom, as in thiophene-, furane-, or pyridine-containing helicenes.[2] In recent years, a repertoire of synthetic strategies was developed to access all monoaza[5]helicenes as well as some diaza[5]helicenes.[3] The properties of these materials are related to the stereodynamics of these helical chiral compounds. By exploration of the unexpected broad range of physicochemical properties of aza[n]helicenes it was realized that there is an opportunity to modulate a specific property by controlled design of the position of the N atoms in the helical molecular frame. In this contribution, we show a complete stereodynamic characterization of monoaza[5]-helicenes combining enantioselective dynamic HPLC and DFT calculations. At variance with previous theoretical calculations[4], 1-aza[5]helicene shows a surprisingly high enantiomerization barrier, which is triggered by specific solvent interactions. [5]

References

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