

Publication

Atropisomerization of di-para-substituted propyl-bridged biphenyl cyclophanes

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)**ID** 1541679**Author(s)** Rotzler, Jurgen; Gsellinger, Heiko; Bihlmeier, Angela; Gantenbein, Markus; Vonlanthen, David; Häussinger, Daniel; Kloppe, Wim; Mayor, Marcel**Author(s) at UniBasel** [Mayor, Marcel](#) ; [Rotzler, Jürgen](#) ; [Gsellinger, Heiko](#) ; [Gantenbein, Markus](#) ; [Vonlanthen, David](#) ; [Häussinger, Daniel](#) ;**Year** 2013**Title** Atropisomerization of di-para-substituted propyl-bridged biphenyl cyclophanes**Journal** Organic and Biomolecular Chemistry**Volume** 11**Number** 1**Pages / Article-Number** 110-8

The influence of electron donors and electron acceptors of variable strength in the 4 and 4' position of 2 and 2' propyl-bridged axial chiral biphenyl cyclophanes on their atropisomerization process was studied. Estimated free energies [$\Delta G^\ddagger(T)$] of the rotation around the central biphenyl bond which were obtained from 1H-NMR coalescence measurements were correlated to the Hammett parameters [σ_p] as a measure for electron donor and acceptor strength. It is demonstrated that the resulting nice linear correlation is mainly based on the influence of the different substituents on the π -system of the biphenyl cyclophanes. By lineshape analysis the rate constants were calculated and by the use of the Eyring equation the enthalpic and entropic contributions were evaluated. Density functional theory calculations show a planar transition state of the isomerization process and the calculated energy barriers based on this reaction mechanism are in good agreement with the experimentally obtained free energies.

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