Synthesis, Structural Analysis, and Chiral Investigations of Some Atropisomers with EE-Tetrahalogeno-1,3-butadiene Core

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Résumé en anglais	The atropenantiomers of stable 1,2,3,4-tetrahalo-1,3-butadiene derivatives (where halogeno stands for bromine or iodine) were separated with use of chiral HPLC. The barriers for the enantiomerization process were determined on-line by dynamic HPLC (DHPLC) or off-line by classical kinetic measurements. In the case of the tetrachloro compound, the barrier was too low for DHPLC and its value was obtained by dynamic NMR experiments. The obtained barriers for chloro, bromo, and iodo derivatives correlate with the van der Waals radii of the halogens. The absolute configuration of the isolated enantiomers of the tetraiodo and tetrabromo compounds was assigned by comparison of the experimental and conformations averaged calculated VCD spectra. The identification of a signature band of the absolute configuration of the butadiene core, the sign and location of which are independent from the different conformations and substituents, allowing the safe assignment of the absolute configuration of the enantiomers of chiral 1,3-butadienes, is also reported.
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