

(E)-4-Methyl-1-tributylstannyl-oct-1-en-6-yn-3-ol: Circular Dichroism Measurement and Determination of the Absolute Configuration by Quantum-chemical CD Calculations

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The chiroptical properties of the diastereomeric alcohols (E)-(3*S*,4*S*)-4-methyl-1-tributylstannyl-oct-1-en-6-yn-3-ol ((*S,S*)-**3**) and (E)-(3*R*,4*S*)-4-methyl-1-tributylstannyl-oct-1-en-6-yn-3-ols ((*R,S*)-**3**) have been studied experimentally as well as by quantum-chemical calculations. The structures of 20 conformers of each isomer, which were found to represent local minima at the MNDO level, have been optimized with density functional theory (DFT). Based on these geometries the excitation energies and oscillator as well as rotational strengths have been calculated using a time-dependent DFT (TDDFT) method. The CD spectra of the compounds were then obtained as superposition of Boltzmann-weighted spectra for each of the structures. By comparison of the calculated and the experimental CD spectra the absolute configurations have been assigned to the investigated compounds.

Key words: Conformational Analysis; Circular Dichroism; TDDFT Calculations.