

Resolution and Determination of the Absolute Configuration of a Twisted Bis-Lactam Analogue of Troger's Base: A Comparative Spectroscopic and Computational Study - DTU Orbit (08/11/2017)

Resolution and Determination of the Absolute Configuration of a Twisted Bis-Lactam Analogue of Troger's Base: A Comparative Spectroscopic and Computational Study

The first reported twisted bis-lactam, a racemic Troger's base (TB) analogue (2), was resolved into its enantiomers on a chiral stationary phase HPLC column. The absolute configuration of (+)-2 was determined to be (R,R)-2 by comparing experimental and calculated vibrational circular dichroism (VCD) and electronic circular dichroism (ECD) spectra. The absolute configuration of (-)-2 was determined by comparing experimental and calculated electronic circular dichroism (ECD) spectra. The corresponding theoretical spectra were calculated using the lowest energy conformation of (R,R)-2 and (S,S)-2 at the B3LYP/6-31G(d,p) level of theory. The absolute configuration of (+)-2 was also determined to (R,R)-2 by anomalous X-ray diffraction (AXRD) in a chiral space group P2(1)2(1)2(1) using Cu-irradiation resulting in a very low Flack parameter of -0.06(3), despite the heaviest element being an oxygen atom, thus unambiguously confirming the results from the spectroscopic studies. We conclude that, for the Troger's base (TB) analogue (2), we may rank the reliability of the individual methods for AC determination as AXRD >> VCD > ECD, while the synergy of all three methods provides very strong confidence in the assigned ACs of (+)-(R,R)-2 and (-)-(S,S)-2.

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