Absolute configuration determination and conformational analysis of (-)-(3s,6s)-3?,6?-diacetoxytropane using vibrational circular dichroism and DFT techniques

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The absolute configuration of semisynthetic (-)-3?,6?- acetoxytropane 1, prepared from (-)-6?-hydroxyhyoscyamine 2, has been determined using vibrational circular dichroism (VCD) spectroscopy. The vibrational spectra (IR and VCD) were calculated using DFT at the B3LYP/DGDZVP level of theory for the eight more stable conformers which account for 99.97% of the total relative abundance in the first 10 kcal/mol range. The calculated VCD spectra of all considered conformations showed two distinctive spectral ranges, one between 1300 and 1200 cm-1, and the other one in the 1150-950 cm-1 region. When compared with the experimental VCD spectrum, the first spectral region confirmed the calculated conformational preferences, whereas the second region showed little change with conformation, thus allowing the determination of the absolute configuration of 1 as (3S,6S)-3?, 6?-diacetoxytropane. Also, the bands in the second region showed similarities between 1 and 2 in both the experimental and calc