CONFORMATIONAL ANALYSIS OF D-ALTROPYRANOSIDE DERIVATIVES

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Due to their low ring inversion barrier, D-altrose derivatives often occur as conformational mixtures of $^4C_1$, $^1C_4$ and other conformations. In addition to NMR spectroscopic and theoretical analysis [1], we have employed vibrational circular dichroism (VCD) [2], which has the potential to serve as a spectroscopic technique for assigning dynamic equilibria of monosaccharide conformations.
We have employed VCD to explore the conformational properties of altrobiosides and of both anomers of *O*-(D-altropyranosyl) trichloroacetimidate showing different conformations [2]. We have been inspired by the work of Taniguchi and Monde who demonstrated that VCD is suitable for distinguishing anomers and moreover for studying carbohydrate conformations [3]. Here, we further demonstrate the potential of VCD for the analysis of sugar conformations, hence complementing other spectroscopic techniques such as NMR.
The VCD of the anomeric *O*-(D-altropyranosyl) trichloroacetimidates are depicted in Figure 1 together with the calculated reference spectra (using the Jaguar software). Weighting of the spectra led to a remarkable agreement between the experimental and calculated spectra. It could be deduced from this data that the α-anomer mainly adopted a $^4C_1$ conformation while the β-anomer showed an equally weighted conformational dynamic between the complementary chairs $^4C_1$ and $^1C_4$.

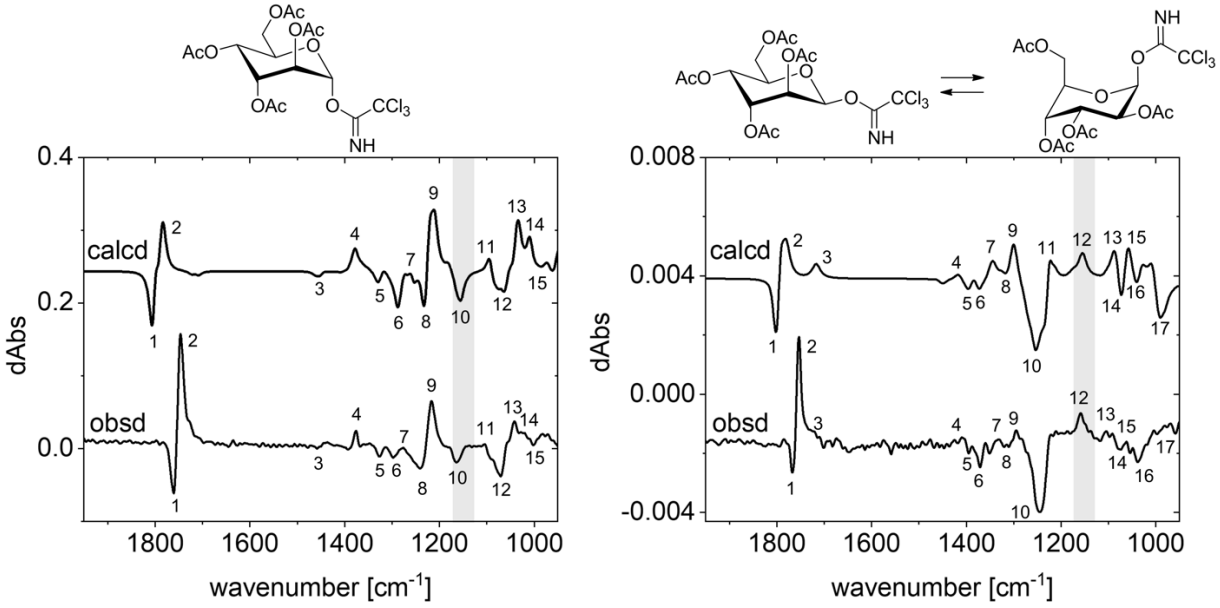

Figure 1. VCD spectra of the anomeric *O*-(D-altropyranosyl) trichloroacetimidates.[2] The VCD bands were numbered accordingly and the glycoside band is highlighted in grey.

References:
1. S. O. Jaeschke, T. K. Lindhorst, A. Auer, *Chem. Eur. J.* **2022**, *28*, e202201544.
2. C. Lütjohann, C. Näther, T. K. Lindhorst, *Carbohydr. Res.* **2024**, *544*, 109228.
3. T. Taniguchi, K. Monde, *Chem. Asian J.* **2007**, *126*, 1258-1266.