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Revisiting an old concept: the coupled oscillator model for VCD. Part 2: Implications of the generalised coupled oscillator mechanism for the VCD robustness concept

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Electronic Supplementary Information

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1 Linear transit calculations for 3,3'-bicamphorylidene

Linear transit calculation have been performed also for the dihedral angle $C^5-C^3-C^{11}-C^{16}$. Fig. 1 shows the variation of the energy during the linear transit scan. The variation of the energy during the LT scan performed for the $O^{49}-C^5-C^{16}-O^{50}$ dihedral angle is also shown in Fig. 1. The VCD spectra computed for the $C^5-C^3-C^{11}-C^{16}$ LT structures -6 to +9 are shown in Fig. 2. As highlighted, during the $C^5-C^3-C^{11}-C^{16}$ LT scan, the expected VCD sign change of the carbonyl stretching bands happens in the LT structures +5 and +8, i.e. significantly later than in the $O^{49}-C^5-C^{16}-O^{50}$ LT scan.





Figure 1: Schematic representation of the 3,3'-bicamphorylidene molecule (upper panel) and energy dependence on the dihedral angle made by the two carbonyl bonds (lower panel). The molecular fragments used in the GCO analysis have been highlighted in red (fragment \mathbf{A}), blue (fragment \mathbf{B}) and black (fragment \mathbf{R}). The LT structures for which VCD calculations have been performed have been highlighted in orange.



Figure 2: Dependence of the computed VCD spectra on the dihedral angle made by the two carbonyl bonds.