

## CHIRAL ISOTOPOLOGUES OF CRYPTOPHANE-B: SYNTHESIS AND CHIROPTICAL PROPERTIES

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Deuterium substitution is the smallest chemical transformation that can be performed on organic compounds. Nevertheless, this simple modification of the structure can change the physical properties of a compound by transforming an achiral molecule into a chiral molecule. Stereochemical analysis, along with synthetic studies of isotopically chiral molecules, have been extremely scarce.<sup>1,2</sup> Thus, the synthesis of isotopologues of cryptophane-B compound (chart 1) represents a challenge as well as the study of their chiroptical properties.

For this oral presentation, we present the synthesis of a chiral isotopologue of cryptophane-B (achiral, chart 1a) whose synthesis has been only recently reported.<sup>3</sup> Strategy used to prepare this compound allows us to synthesize a chiral isotopologue (chart 1b) by replacing three methoxy group by three deuterium labelled methoxy groups. The two enantiomers of this new compound have been isolated and their chiroptical properties have been investigated by electronic circular dichroism (ECD), vibrational circular dichroism (VCD) and Raman optical activity (ROA) spectroscopy. Specific spectral signatures have been measured by ECD, VCD and ROA for the two enantiomers of this isotopologue.

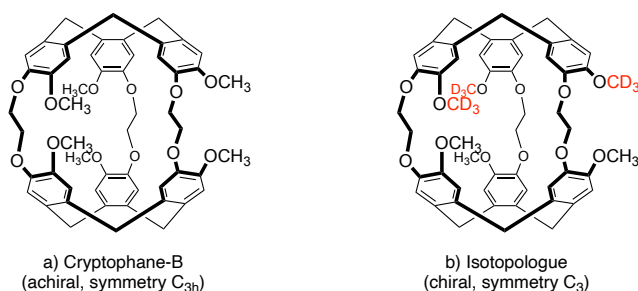


Chart 1: Chemical structures of cryptophane-B and its isotopologue.

### REFERENCES:

1. J. Haesler, et al. *Nature* **2007**, 446, 526.
2. T. Miura, et al. *Angew. Chem. Int. Ed.* **2017**, 56, 3334.
3. T. Brotin, et al., *J. Org. Chem.* **2018**, 83, 14465.

**KEYWORDS:** Cryptophanes, Isotopologues, Chirality, VCD, ROA