Unveiling the conformational dynamics of Binaphthols in their excited state by ultrafast circular dichroism

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Axially chiral molecules, such as 1,1′-bi-2-naphthols (binols), have attracted a great deal of interest, these past decades. Binols have been widely used as chiral templates for the synthesis of a large variety of chiral sensors for applications in catalysis and molecular recognition.[1-4]. Axial chirality of binols gives them strong chiroptical activity providing interesting perspectives for applications in the fields of non-linear optics and optoelectronics.[5-9] In this context, a deeper understanding of the photoinduced changes in their chirality is desirable. While significant efforts have been devoted to understanding the chiroptical properties of hindered binaphthyls in the ground state,[10,11] their fate in the excited state have been rarely addressed, so far.[12,13]

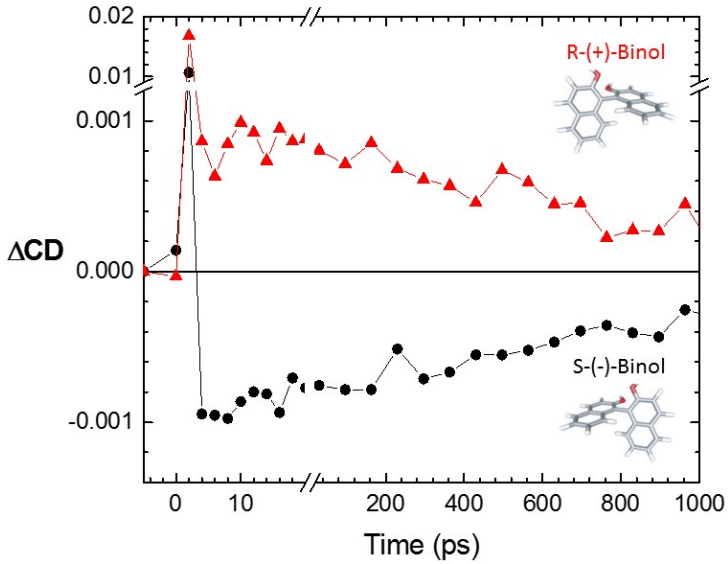

Figure 1. CD changes in (R) and (S) enantiomers of binol measured in ethanol at 234 nm, after 500-fs excitation at 266 nm.

In order to provide a comprehensive analysis of the parameters that govern chirality and the associated conformational changes of biaryls in their excited state, we undertook a comparative study of binol (Fig.1) with several bridged derivatives in different solvents by

time-resolved circular dichroism (TRCD) with a sub-picosecond time resolution. In contrast with transient absorption, TRCD provides a direct information about the conformational changes of binols. These measurements allowed us to disentangle the respective effects of the solvent and the substituents on the chirality of hindered binaphthyls in their excited-state. We interpret our results in the frame of the exciton model developed by Masson et al.[10,11]

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