Accepted Manuscript

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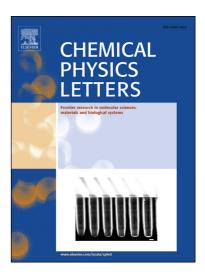
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PII: S0009-2614(17)30243-9

DOI: http://dx.doi.org/10.1016/j.cplett.2017.03.023

Reference: CPLETT 34623

To appear in: Chemical Physics Letters



Please cite this article as: C. Consani, M. Berberich, F. Würthner, T. Brixner, Ultrafast isomerization in a difluoroboryl-coordinated molecular switch, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.03.023

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ACCEPTED MANUSCRIPT

Ultrafast isomerization in a difluoroboryl-coordinated molecular switch

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Abstract

Molecular switches based on light-induced isomerization cycles are promising materials for sensors and biomedical applications. Understanding the details of the isomerization photocycle and identifying the nuclear coordinates involved in the photoreaction are relevant topics. Here we characterize the $cis \rightarrow trans$ and $trans \rightarrow cis$ isomerization of a new type of BF₂-coordinated azo-dye molecular switch by pump-probe spectroscopy. While $cis \rightarrow trans$ isomerization is ultrafast and proceeds via a conical intersection, the $trans \rightarrow cis$ photocycle is more complex and involves at least three reaction channels. Finally, we employ the vibrational wavepackets accompanying isomerization to infer information on the nuclear degrees of freedom involved in the photoreaction.

Keywords:

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