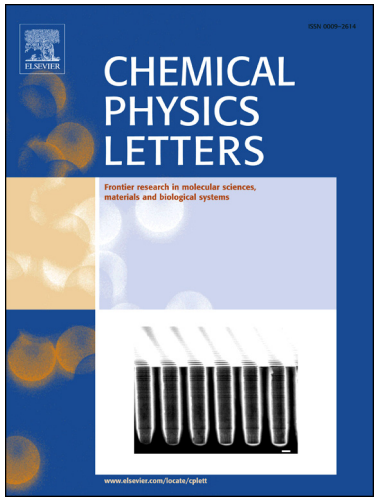

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Ultrafast isomerization in a difluoroboryl-coordinated molecular switch

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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*→*trans* and *trans*→*cis* isomerization of a new type of BF_2-coordinated azo-dye molecular switch by pump-probe spectroscopy. While *cis*→*trans* isomerization is ultrafast and proceeds via a conical intersection, the *trans*→*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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