MS50.O04

Photochromism in a New Light: Temperature-Dependent in situ Photocrystallography

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Organic photochromic molecules including diarylethenes are of particular interest for their potential applications in fields of high density optical data storage and light-activated switches, among many others. However, one of the limitations in diarylethene-based systems has been the low photoconversion observed in neat single crystals which is often less than 20%. The low conversion is typically believed to be the result of screening effects in which the photoisomerized molecules at the surface absorb incident light preventing full isomerization of the crystal. To assess the effect of screening on a model diarylethene system, photocrystallographic experiments on microcrystals of the compound were performed using synchrotron radiation at the Advanced Photon Source at Argonne National Labs. During the course of the study, we discovered that the photoconversion of the diarylethene crystals exhibits highly unusual temperature dependent behavior which is incongruent with current computational models of diarylethene photochemistry. Herein we report the first temperature-dependent 'constant irradiation' in situ photocrystallography experiments performed on a photochromic system. Through the application of this technique, combined with spectroscopic analysis, we demonstrate that the steady-state population arising from the photo-cyclization reaction shows a temperature dependence which has been heretofore unobserved. Possible explanations for this anomalous behavior and its role in the photochemical reactivity of this and other diarylethene systems will be presented.

Keywords: Diarylethene, Photocrystallography, Temperature-dependent