Generation of an usually stable merocyanine via a unique mechanochemical reaction pathway

Molly McFadden¹, Maxwell J. Robb¹

1. Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, United States.

A wide range of force-coupled reactions have been developed since the emergence of the contemporary field of polymer mechanochemistry around 2005. Discovery of new mechanochemical transformations expands both the range of applications for force-responsive materials and the fundamental understanding of force-mediated reactivity. Naphthopyrans are mechanophores that undergo a reversible 6 electrocyclic ring-opening reaction under force to generate intensely colored merocyanines. Thermal electrocyclization often occurs under ambient conditions, resulting in loss of color. The naphthopyran mechanophore has been successfully derivatized to access mechanochromic polymers with variable colors, fading rates, and even force-dependent multicolor responses. However, to date, all naphthopyran mechanophores belong to a structural family known for particularly rapid thermal reversion. We recently discovered a new class of mechanochemically active naphthopyrans that generates an unusually stable merocyanine dye under mechanical force. Excitingly, the remarkable stability of this merocyanine is unique to the mechanochemical reaction pathway and is not accessed under photochemical activation. We discuss the elucidation of a novel force-mediated transformation and the identification of the unusual merocyanine product, and the potential impact of this new mechanochromic mechanophore in stress-reporting polymers.

