The Effect of Regiochemistry on Naphthopyran Mechanochromism

Abigail J. Halmes and Jeffrey S. Moore

The mechanophore hypothesis states that force drives chemical change in selective and productive ways. Previous work in the field has demonstrated multiple structures, known as mechanophores, which undergo chemical change in response to mechanical force when incorporated into a polymer matrix. New structures are hypothesized and investigated largely based upon intuition and similarities to known mechanophores. There is a need for a more efficient design protocol. Naphthopyran based compounds have been widely studied due to their UV-triggered reversible color changing-properties. We have previously shown that one regioisomer of 3H-naphtho[2,1-*b*]pyran acts as a color-changing mechanophore. Here we report the effect of increasing the angle between the direction of force application and the mechanochemically active bond on the properties of the full series of naphthopyran regioisomers. Using both DFT calculations and experimental methods we identify three mechanophores in the series of six regioisomers. The structure-property relationship informs the development of principles that will guide the rational design of future mechanophores.