Push–Pull Chromophores from Indan-1,3-dione

Modification of indan-1,3-dione:

\[
\begin{align*}
\text{Indan-1,3-dione} & \xrightarrow{\text{I}_2, \text{H}_2\text{SO}_4 \text{ (fuming), 70 °C}} \text{Iodinated indan-1,3-dione} \\
& \xrightarrow{\text{1. ethyl acetoacetate, } \text{Et}_3\text{N, Ac}_2\text{O, 25 °C}, \text{50% yield}} \text{Ethyl acetoacetate adduct} \\
& \xrightarrow{\text{2. HCl-H}_2\text{O, 80 °C}, \text{50% yield}} \text{Iodinated indan-1,3-dione} \\
& \xrightarrow{\text{Pd-catalyzed cross-coupling, } \text{n = 0, 80% yield, } n = 1, 77% \text{ yield}} \text{T-Shaped chromophore}
\end{align*}
\]

T-Shaped chromophore synthesis:

**Significance:** The synthesis of T-shaped push–pull chromophores based on indan-1,3-dione as an electron acceptor is presented. The two donor moieties that comprise the T-shaped architecture are installed via the Knoevenagel condensation of 4,7-diiodoindan-1,3-dione with an aryl aldehyde, followed by palladium-catalyzed cross-coupling of the iodides with \(N,N\)-dimethylaniline or thiophene-containing substituents.

**Comment:** The optical and electronic properties of the synthesized T-shaped chromophores are extensively studied by UV/Vis absorption spectroscopy and calculations. Their non-linear optical properties are also examined through theoretical calculations.