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

Modification of indan-1,3-dione:

\[
\begin{align*}
\text{I}_2 & \xrightarrow{\text{H}_2\text{SO}_4 \text{ (fuming), 70 °C}} \text{46% yield} \\
\text{1. ethyl acetoacetate} & \xrightarrow{\text{Et}_3\text{N}, \text{Ac}_2\text{O, 25 °C}} \\
\text{2. HCl-H}_2\text{O, 80 °C} & \xrightarrow{50\% \text{ yield}} \\
\end{align*}
\]

T-Shaped chromophore synthesis:

\[
\begin{align*}
\text{Pd-catalyzed} & \xrightarrow{\text{cross-coupling}} \\
n = 0, 82\% \text{ yield} & \quad n = 1, 60\% \text{ yield} \\
n = 0, 47\% \text{ yield} & \quad n = 1, 75\% \text{ yield} \\
n = 0, 32\% \text{ yield} & \quad n = 1, 74\% \text{ yield} \\
\end{align*}
\]

**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.