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

Modification of indan-1,3-dione:

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

T-Shaped chromophore synthesis:

\[
\begin{align*}
Pd\text{-catalyzed cross-coupling} & \\
\text{N} & \quad \text{Me} \\
\text{Me} & \\
\text{R} & \\
\text{Me} & \quad \text{N} \\
\text{Me} & \\
\end{align*}
\]

**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.