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

Modification of indan-1,3-dione:

\[
\begin{align*}
\text{I}_2 & \quad \text{H}_2\text{SO}_4 \text{ (fuming)}, \ 70 \ ^\circ\text{C} \\
\text{O} & \quad \text{O} \\
\text{I}_2 & \quad \text{HCl–H}_2\text{O}, \ 80 \ ^\circ\text{C} \\
\text{O} & \quad \text{O} \\
\text{Me} & \quad \text{N} \\
\text{Me} & \quad \text{Me} \\
\text{R} & = \text{S} \\
\end{align*}
\]

T-Shaped chromophore synthesis:

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

**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.