Synthesis of tetraaryl-1,4-dihydropyrrrolo-[3,2-b]pyrroles derivatives using niobium pentachloride

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Heteropentalenes are aromatic compounds with 10π delocalized electrons in its structure. That characteristic make these compounds potential candidates as sensitizing dyes of organic electronic devices. Thieno[3,2-b]thiophene is a commercial available product that is used as basis for new compounds with the heteropentalene structure. The pyrrolo-[3,2-b]pyrroles derivatives are scarcely studied as sensitizing dyes in organic electronic devices.

Recently, a synthesis route was described for tetraaryl-1,4-dihydropyrrrolo-[3,2-b]pyrroles derivatives (4a-h) through a multicomponent reaction between 2 moles of aldehydes derivatives, 2 moles of aniline derivatives and 1 mol of butanedione in the presence of acetic acid at 100ºC, with low yields (5-34%).

Based on that, and in the objectives of our research group of applying the niobium compounds as catalyst in organic synthesis, we carried out the synthesis of tetraaryl-1,4-dihydropyrrrolo-[3,2-b]pyrroles derivatives using niobium pentachloride as catalyst for the pentacomponent reaction among toluidine (1), benzaldehyde derivatives (2a-h), and 2,3-butanedione (3). The reactions proceeded in room temperature and in anhydrous solvent (CH₃CN). We could synthesize the products in a good reaction time (20-90 min) and with very good yields (49-98%). The products were purified by recrystallization and characterized by spectroscopic and spectrometric methods.

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\begin{align*}
2 + 2 \rightarrow \text{NbCl}_5

1 & \quad R=H & 2a, R=H \\
2b & \quad R=\text{Me} & 2b & \quad R=\text{Me} \\
2c & \quad R=\text{OMe} & 2c & \quad R=\text{OMe} \\
2d & \quad R=F & 2d & \quad R=F \\
2e & \quad R=\text{Cl} & 2e & \quad R=\text{Cl} \\
2f & \quad R=\text{Br} & 2f & \quad R=\text{Br} \\
2g & \quad R=\text{i-But} & 2g & \quad R=\text{i-But} \\
2h & \quad R=\text{SMe} & 2h & \quad R=\text{SMe}
\end{align*}
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4a-h