



High-efficiency Pyrrole Synthesis (20150075, Dr. Ian Tonks)

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Unprecedented Pyrrole Yield

A newly developed technology for synthesizing polysubstituted pyrroles employs a titanium-catalyzed reaction of alkynes and diazenes to form the substituted pyrrole. The process, which uses an early transition metal catalyst and works through a 3-component formal [2+2+1] oxidative coupling of alkynes and diazenes, can catalyze cyclization with unprecedented atom efficiency and reaction yield for pyrrole formation. This process has a high conversion rate, high selectivity and can synthesize compounds containing variety of alkyl and aromatic side chains.

Alternative to Paal-Knorr Reaction

Pyrroles and derivatives are structurally important heterocycles used in pharmaceuticals, natural products, dyes and conducting polymers. Synthesizing polysubstituted pyrroles is often challenging and current methods, like the Paal-Knorr reaction, often result in low atom economy, in which two oxygen atoms are lost per pyrrole ring produced and/or two water molecules are released as a byproduct. This new catalytic method results in 100% atom efficiency during the pyrrole ring formation reaction and delivers greater than 90% product yield.

BENEFITS AND FEATURES OF HIGH-EFFICIENCY PYRROLE SYNTHESIS:

- 100% atom economy; no byproducts created
- Unprecedented pyrrole yield (greater than 90%)
- Catalytic reaction fueled by cost-effective, earth-abundant and nontoxic titanium
- High conversion rate and high selectivity
- May synthesize pyrroles with a variety of alkyl and aromatic side chains
- Used for synthesis of fine- and industrial-grade feedstock chemicals

Phase of Development - Proof of concept

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