



## Technology Offer

## Air-Stable Molybdenum Alkylidyne Catalysts for High Performance Alkyne Metathesis

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## Background

During the past two decades, alkyne metathesis has arguably evolved from a curiosity to a method of strategy level status in material science and small molecule synthesis. Notwithstanding the high level of sophistication in the field, improved user-friendliness is desirable; only if the best catalysts are easy to handle are they going to be routinely used. Thus the development of efficient and stable catalysts for this reaction is crucial for enabling more sustainable and versatile synthetic pathways.

## Technology

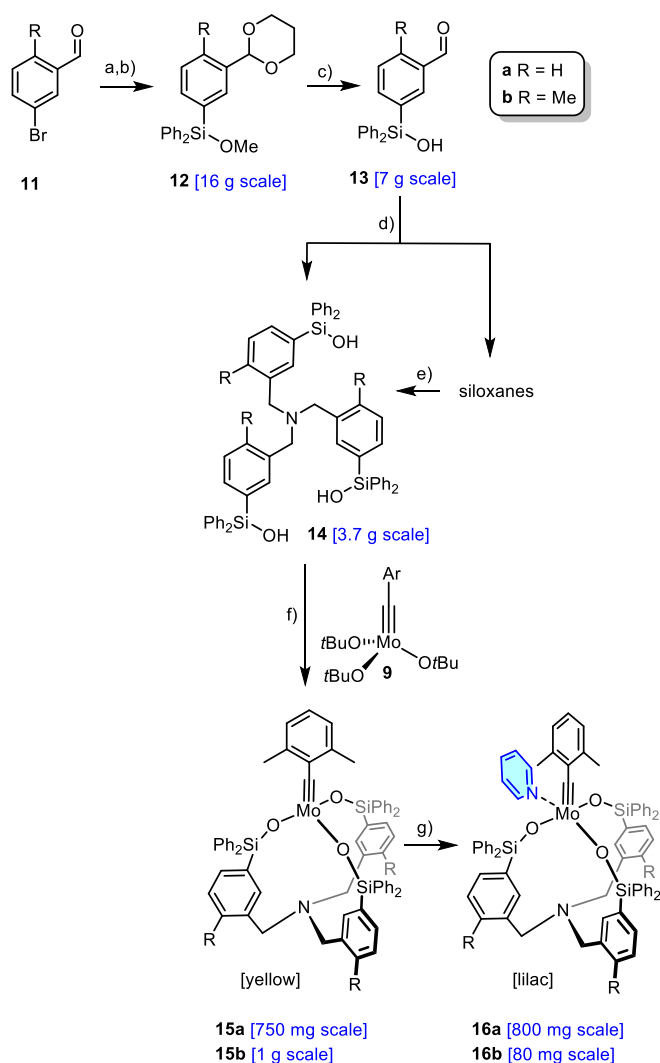
Prof. Alois Fürstner and co-workers at the Max Planck Institut für Kohlenforschung have developed a new class of molybdenum alkylidyne catalysts with tripodal silanolate ligands. These catalysts are designed for improved stability and functional group tolerance, and are easy to synthesize on a gram scale.

The new catalysts meet all critically important aspects: the pyridine adducts **16** can be routinely weighed and handled in air, and can be stored for long periods outside a glove box, for example in a desiccator.

When dissolved in toluene, however, spontaneous dissociation of the stabilizing pyridine ligand releases an active species of excellent performance and functional group tolerance.

This active species meets the highest standards of reactivity and selectivity, encompassing a wide range of polar and apolar functional groups and different protic sites, as well as numerous basic functionalities. These chemical virtues are all the more remarkable as the operative unit is an early transition metal in its highest oxidation state.

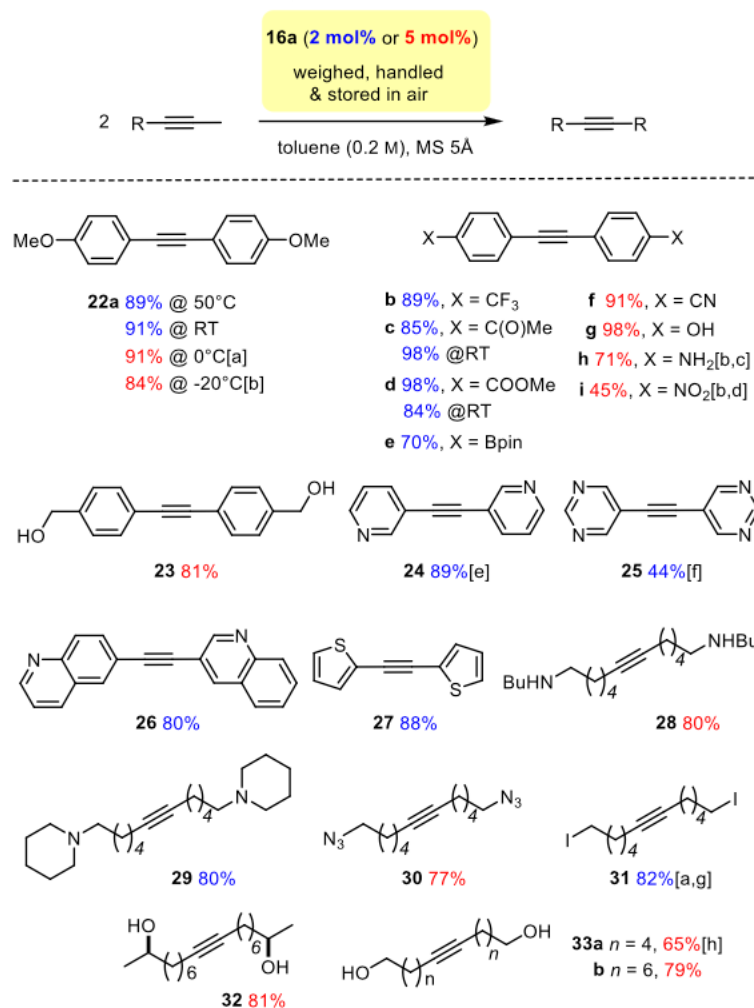
## Scheme 1. of Ligands and Catalysts





A detailed performance evaluation confirmed the broad functional group tolerance of **16**. These new user-friendly catalysts are active in the presence of primary and secondary aliphatic, benzylic and propargylic alcohols, a phenolic -OH, the -NH<sub>2</sub> substituent of an aniline, and the -NH group of a secondary amine. Various donor sites and heterocycles are tolerated.

A number of successful ring closing alkyne metathesis reactions with formation of macrocyclic rings and advanced natural product syntheses reinforce the positive impression with regard to the catalytic performance. The list includes a precursor for the anticancer drug epothilone C (detailed information in the JACS publication below).



**Scheme 2.** Homo-metathesis Reactions of Functionalized Substrates Using Complex **16a** as the catalyst at 50°C, unless Stated Otherwise;  
the Catalyst Loading Is Color-Coded (Blue = 2 mol%; Red = 5 mol%)

### Literature

Alois Fürstner et al: "From the Glovebox to the Benchtop: Air-Stable High Performance Molybdenum Alkylidyne Catalysts for Alkyne Metathesis", J. Am. Chem. Soc. 2023, 145, 26993–27009

### Patent Information

EP priority patent application filed in August 2023.

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