

Demonstrating Reactivity of Terminal Mo Carbides

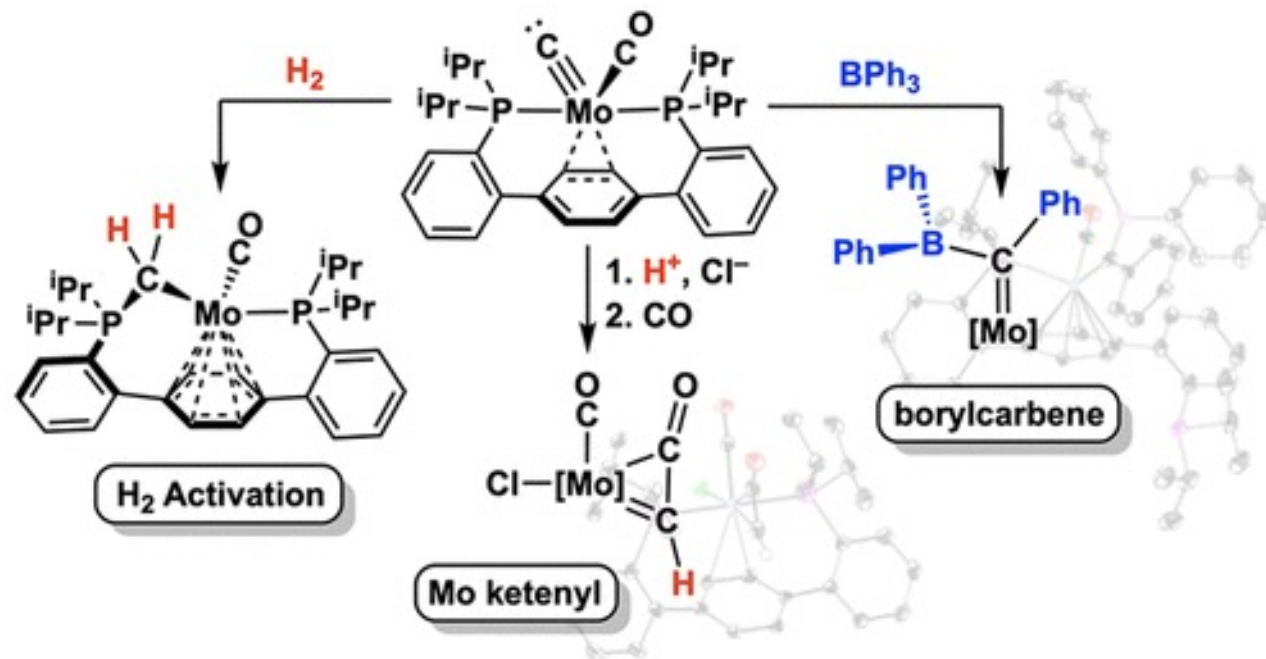
Gwendolyn A. Bailey and Theodor Agapie*, "Terminal Mo Carbide and Carbyne Reactivity: H₂ Cleavage, B-C Bond Activation, and C-C Coupling," *Organometallics* 2021, 40, 2881.

Scientific Achievement

- Terminal metal carbides may be involved as intermediates in fuel-forming reactions from CO and CO₂, but they are rare in molecular form
- Here we probe the reactivity of a terminal Mo carbide with H₂ and Lewis acids

Significance and Impact

- Fundamental understanding of carbide reactivity could lead to new methods for converting CO₂ or CO and H₂ into sustainable liquid fuels



Bond activation and C-C coupling reactions starting from a terminal Mo carbide. Reprinted with permission from *Organometallics*. Copyright 2021 American Chemical Society.

Technical Details

- Reaction of Mo carbide with H₂ leads to carbide hydrogenation
- Reaction with BPh₃ results in B-C bond cleavage
- After protonation to the methylidyne, C-C coupling is observed to a rare terminal Mo-ketenyl complex
- B-C bond cleavage by the carbide yields an unusual example of a Mo-borylcarbene bearing a direct Mo-B contact.