

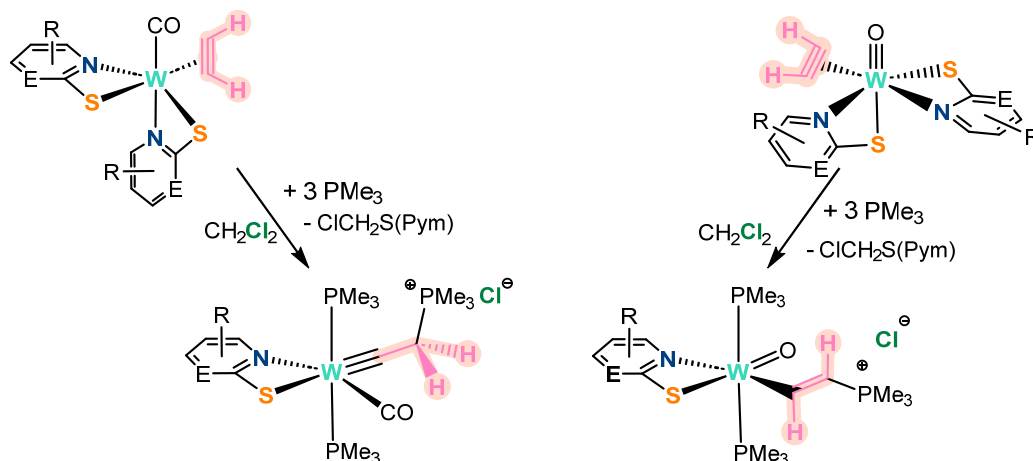
FROM NATURE TO ORGANOMETALLIC CHEMISTRY – INSIGHTS INTO THE MECHANISM OF ACETYLENE HYDRATASE

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Molybdenum and tungsten are the only 2nd and 3rd-row transition metals known to be essential in biology. Both enable the transfer of an oxygen atom in various reactions. Tungsten-dependent acetylene hydratase (AH) catalyzes the net-hydration reaction of acetylene to acetaldehyde. Two diverging mechanisms are discussed in the literature: it is unclear which of the two substrates, water or acetylene, is coordinated at tungsten within the active site during the catalytic cycle.

We develop bioinspired model chemistry, which leads us one step further towards a mechanistic understanding of the enzymes AH. The tungsten complexes supported by sulfur-rich ligands, such as pyridine-2- or pyrimidine-2-thiolates, allow the coordination of acetylene and their subsequent nucleophilic attack.[1] This presentation will highlight the influence of the oxidation state on product formation. Detailed mechanistic studies by synthetic, spectroscopic, and theoretical efforts emphasize the importance of the observed tungsten(IV) in the active site of acetylene hydratase.



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[1] Madeleine A. Ehweiner, Lydia M. Peschel, Niklas Stix, Miljan Z. Ćorović, Ferdinand Belaj, and Nadia C. Mösch-Zanetti *Inorg. Chem.* **2021**, *60*, 8414–8418.