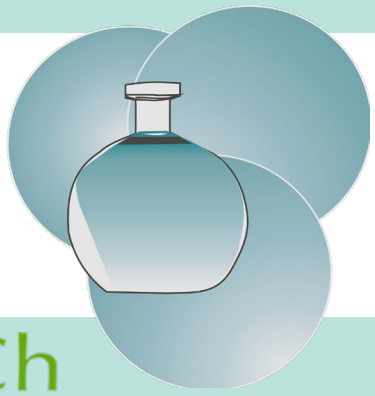
Fakultät für Naturwissenschaften

Institut für Chemie



lädt ein

gemeinsam mit der Gesellschaft Deutscher Chemiker zum

Vortrag

von Herrn

Prof. Warren Piers

University of Calgary
Department of Chemistry

Gesellschaft Deutscher Chemiker

“Molybdenum Complexes for Ammonia Activation: Mechanisms of Hydrogen Production and N-N Bond Formation.”

am: 13. Oktober 2023

um: 16:00 Uhr

wo: im Raum 1/232

Achtung!
Dieser Vortrag findet freitags statt.

Die kleine Kaffeerunde vor dem Vortrag beginnt um 15:30 Uhr im Raum 1/232.
Das Mitbringen von eigenen Trinkgefäßen ist erwünscht.

Gäste sind herzlich willkommen!

TECHNISCHE UNIVERSITÄT
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Fakultät für Naturwissenschaften

Institut für Chemie

Prof. Warren Piers

University of Calgary
Department of Chemistry

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"Molybdenum Complexes for Ammonia Activation: Mechanisms of Hydrogen Production and N-N Bond Formation."

Ammonia oxidation catalyzed by molecular compounds is of current interest as a potentially carbon free source of dihydrogen. Two key processes in this complex reaction are the activation of N-H bonds through coordination induced bond weakening at transition metal centers and N-N bond formation from various MNH_n (n = 0-2) intermediates. In this talk, we report the substantial N-H bond weakening in coordinated ammonia *via* reaction with low valent Mo complexes of a diborate pentadentate ligand system. Spontaneous loss of hydrogen atoms from $(B_2Pz_4Py)Mo(II)\text{-}NH_3$ at room temperature to produce H_2 and the dinuclear μ-nitrido compound $(B_2Pz_4Py)Mo\text{-}N\text{-}Mo(B_2Pz_4Py)$ is observed upon coordination to Mo. Mechanistic details are supported through the experimental observation and characterization of terminal amido, imido and nitrido complexes. Density functional theory computations provide support for a proposed mechanism for the stoichiometric conversion of $(B_2Pz_4Py)Mo(II)\text{-}NH_3$ to one equivalent of NH_3 to H_2 and the dinuclear μ-nitrido, revealing the role of these bridging nitrido species in potential ammonia oxidation catalytic schemes. Conditions that avoid these thermodynamic sinks and encourage N-N bond formation through bimolecular coupling of terminal MoN derivatives will also be discussed.

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