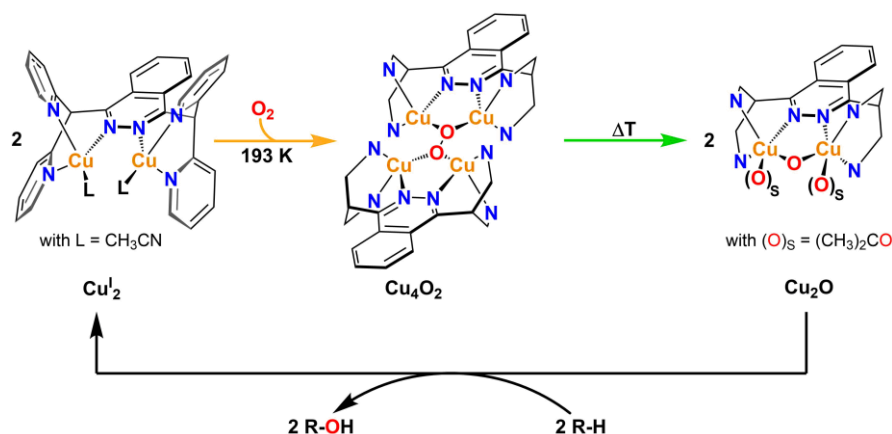


## Model systems of copper-containing monooxygenases with pyridazine backbone

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The activation of C-H bonds by copper enzymes is a subject of high current interest. We have synthesized two catalytically active dinuclear copper complexes supported by hexadentate ligands with pyridazine or phthalazine backbones that bind oxygen and activate it for insertion into the C-H bonds of hydrocarbons. Using a combination of UV/vis, resonance Raman and X-ray absorption spectroscopy as well as mass spectrometry, we were able to understand the fate of oxygen in our model systems, from its initial binding to the copper centers until its final incorporation into aliphatic substrates. The structure of the complexes and the reactive cycle are shown in the Figure.<sup>1</sup>



If exposed to dioxygen, these systems ultimately generate copper complexes with mono- $\mu$ -oxo cores. Due to the special environment, these species are highly electrophilic and able of HAT followed by O-transfer. Recently we have investigated the effect of changing the electronic and geometric properties of the above complexes by modification of the terminal donor groups and the connectivity to the central pyridazine unit. This generated a series of new dinuclear copper complexes allowing the targeted generation of various copper-dioxygen adducts. The electronic and geometric structures of these intermediates and their reactivities towards various aliphatic substrates are discussed.<sup>2</sup>

<sup>1</sup> R. Jurgeleit, B. Grimm-Lebsanft, B. M. Flöser, M. Teubner, S. Buchenau, L. Senft, J. Hoffmann, M. Naumova, C. Näther, I. Ivanović-Burmazović, M. Rübhausen, F. Tuczek *Angew. Chem. Int. Ed.*, **2021**, *60*, 14154 – 14162

<sup>2</sup> R. Jurgeleit, A. Stüber, B. Grimm-Lebsanft, M. Teubner, S. Buchenau, L. Senft, M. Naumova, Y. Appiarius, C. Näther, I. Ivanović-Burmazović, M. Rübhausen, F. Tuczek *manuscript in preparation*