

C–C Bond Formations catalyzed by [NiFe]hydrogenase Functional Models Using H₂ as an Electron Source

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Hydrogen, being producible from renewable energy sources, is an essential energy source for realizing a carbon-neutral society. Hence, there is a growing demand for diverse ways to utilize hydrogen. In the synthesis and conversion of hydrocarbon compounds, hydrogen has been mainly used as hydrogen atom (H•) or hydride ion (H⁻) for hydrogenations and hydrogenative C–C bond formations (Figure 1a).¹ On the other hand, the methodology to use hydrogen as an electron source has not been developed because there are very few catalysts that can extract electrons from hydrogen and use them for C–C bond formations. In nature, [NiFe]hydrogenase extracts electrons from hydrogen and transfers them to an electron acceptor via hydride species and low-valent species (Figure 1b).² We have aimed to mimic this function of [NiFe]hydrogenase and applied it for C–C bond formation using H₂ as an electron source. In this presentation, we demonstrate reductive C–C coupling reactions and C–H arylations using hydrogenase functional models and hydrogen.^{3,4}

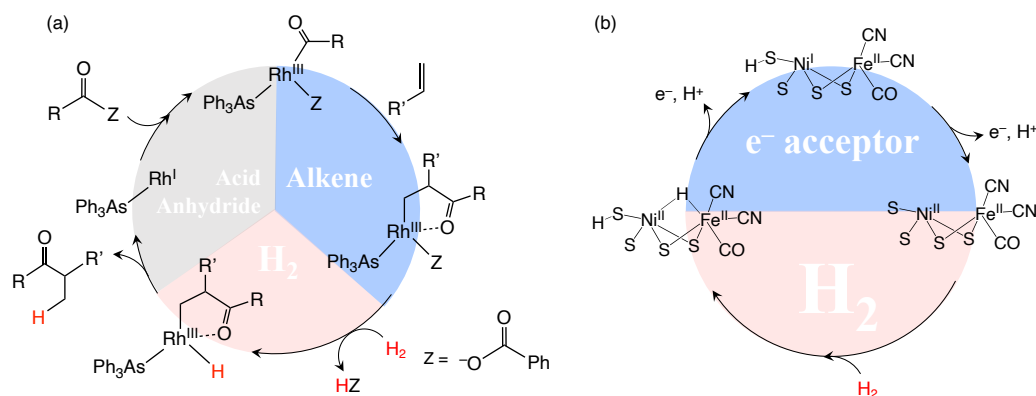


Figure 1. (a) Hydrogenative C–C coupling reaction. (b) H₂ oxidation mechanism of [NiFe]hydrogenase.

References

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