OLEFIN METATHESIS WITH BASE METALS

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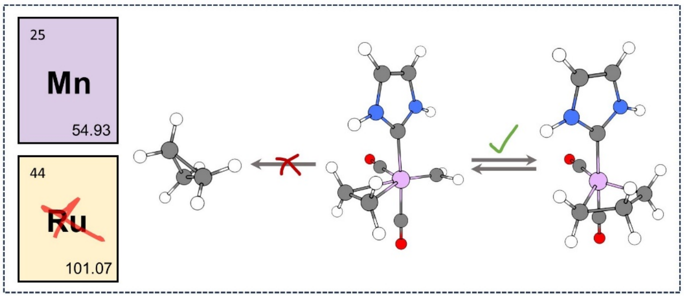
Olefin metathesis is an important process in organic chemistry that demonstrates efficient homogeneous catalysis. While common catalysts employ 4d and 5d metals, first-row transition metals such as iron also allow for cycloaddition and cycloreversion reactions. Surprisingly, despite its relevance in homogeneous catalysis and similarity to Ru(II), the potential of Mn(I) catalysts for olefin metathesis remains untapped. In this study, we investigate Mn complexes for cycloaddition and reversion using density functional theory, focusing on synthetically feasible octahedral carbonyl complexes. Similar to iron, Mn catalysts require a singlet ground state to enable metathesis and avoid unwanted cyclopropanation. Achieving this state requires careful selection of sigma-donor and pi-acceptor properties, with bidentate ligands plus CO showing promising results. Our results highlight the potential of Mn(I) complexes as olefin metathesis catalysts and support their isodiagonal relationship.[1]



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[1] Pecak, J.; Talmazan, R. A.; Kirchner, K.; Podewitz, M. Keep it singlet – Towards in silico design of manganese catalysts for olefin metathesis. Manuscript in preparation.