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Synthesis and reactivity of (Pybox)Os and (Pybox)Ru complexes: Comparison with isoelectronic (Phebox)Ir complexes

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Our laboratory has reported that (CX^3 Pybox)Ir(H)(OAc) (X = H, F) catalysts are highly active for the acceptorless dehydrogenation of n-alkanes¹, particularly in the presence of Lewis acids. In this work we report the synthesis of isoelectronic (Pybox)Os(H)(OAc) and (Pybox)Ru(H)(OAc), and investigation of these complexes for alkane dehydrogenation. DFT calculations predict (Pybox)Ru(H)(OAc) to catalyze acceptorless alkane dehydrogenation with a barrier lower than that for (CH^3 Pybox)Ir(H)(OAc), while the barrier calculated for (Pybox)Os(H)(OAc) is even lower. The rate-limiting step chem. for the catalytic cycle is calculated to be a net M-H/C-H σ -bond metathesis reaction, although expulsion of H₂ from the reaction mixture was found to be rate-determining under typical conditions for acceptorless n-alkane dehydrogenation catalyzed by (CF^3 Pybox)Ir(H)(OAc). H/D exchange experiments were used to probe the kinetics of C-H activation yielding the order of activity: (Pybox)Os(H)(OAc) > (Pybox)Ru(H)(OAc) > (CF^3 Pybox)Ir(H)(OAc). Exptl. investigation of catalysis by (Pybox)Ru(H)(OAc) and (Pybox)Os(H)(OAc) is still in progress but the Ru complex, unfortunately, does not appear to be stable at the high temperatures required for acceptorless alkane dehydrogenation. We have also reported that (CH^3 Pybox)Ir(C₂H₄)₂ catalyzes selective dehydrogenative coupling of ethylene to butadiene via an iridacyclopentane complex.² In this work we used the precursor (Pybox)OsH₄ to investigate the same catalytic reaction and appears to result in an analogous dehydrogenative coupling of ethylene to form butadiene via an osmacyclopentane.

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