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HOW TO DESIGN A BI-FUNCTIONAL MOLECULAR CATALYST FOR HYDROGEN PRODUCTION FROM METHANOL?

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We have studied the mechanism of hydrogen production from methanol by two different and well known ruthenium based molecular catalysts: Ru(trop)2dad complex and pincer supported Ru-PNP complex using density functional theory (DFT) in conjunction with *ab initio* molecular dynamics studies (AIMD) with explicit solvation. The results show that while methanol dehydrogenation occurs via a Noyori type (Ru-N) bi-functional mechanism by the Ru(trop)2dad catalyst, the RuPNP complex does not feature the commonly assumed (Ru-N) bifunctional mechanism under the applied reaction conditions. Ru(trop)2dad catalyst does not require any additive (base/Lewis acid) for activity while the RuPNP complex requires 8M KOH for optimal activity. Several other well-known molecular catalysts also require an additive (base/Lewis acid) for hydrogen production from methanol. Therefore, the mechanistic studies on Ru(trop)2dad and RuPNP systems, and the sharp contrast in their respective mechanistic pathways provide guidelines for rational design of additive free and highly active bi-functional catalysts for hydrogen production from methanol. Moreover, these case studies show the importance of an explicit consideration of solvent molecules for realistic computational modelling of minimum energy reaction pathway.

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