

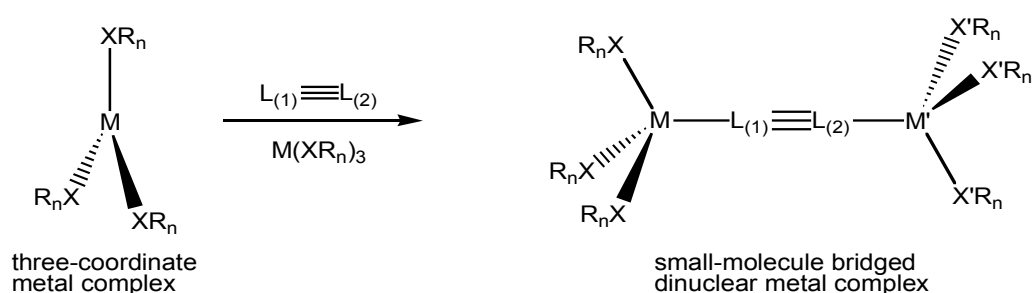
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Note: No prior experience in computational chemistry is required to undertake the project described below.

Activation and Cleavage of Small Multiply-Bonded Molecules.

The industrial processes for activating and cleaving small molecules with very strong multiple bonds such as N_2 and CO , are expensive and require very high temperatures and pressures to induce bond cleavage. Recently, dinuclear metal systems based on sterically-hindered, three- and four-coordinate transition metal complexes of the type $(R_nX)_mM$, where the R_nX ligands comprise bulky organic substituents R , have shown great promise synthetically for the activation and scission of small, multiply-bonded molecules under mild conditions.



This project will use state-of-the-art computational methods to design either three- or four-coordinate transition metal complexes which are specific for binding and activating small molecules such as N_2 , CO and NO , and will involve calculating the structures and energies of the relevant species along the reaction path in order to determine the extent of small molecule activation and the overall reaction energetics.