# Free Energy of Catalytic Reactions by Density Functional Theory

- Interactions of transition metals with organic ligands are very important in a number of catalytic contexts.

- For rational catalyst design, density functional theory (DFT) is widely used to understand metal-ligand binding, but commonly used functionals often have errors of 5 kcal/mol or more.

- Methods developed at Minnesota have been applied for the oxidative addition reaction of a Ir•pentene complex with ammonia. Our calculations employing the M06-L density functional and the SMD solvation model reproduce the experimental free energy of reaction well.

ΔG_{exp} = -1.3 kcal/mol

Hydrogen atoms on carbon atoms are omitted for clarity
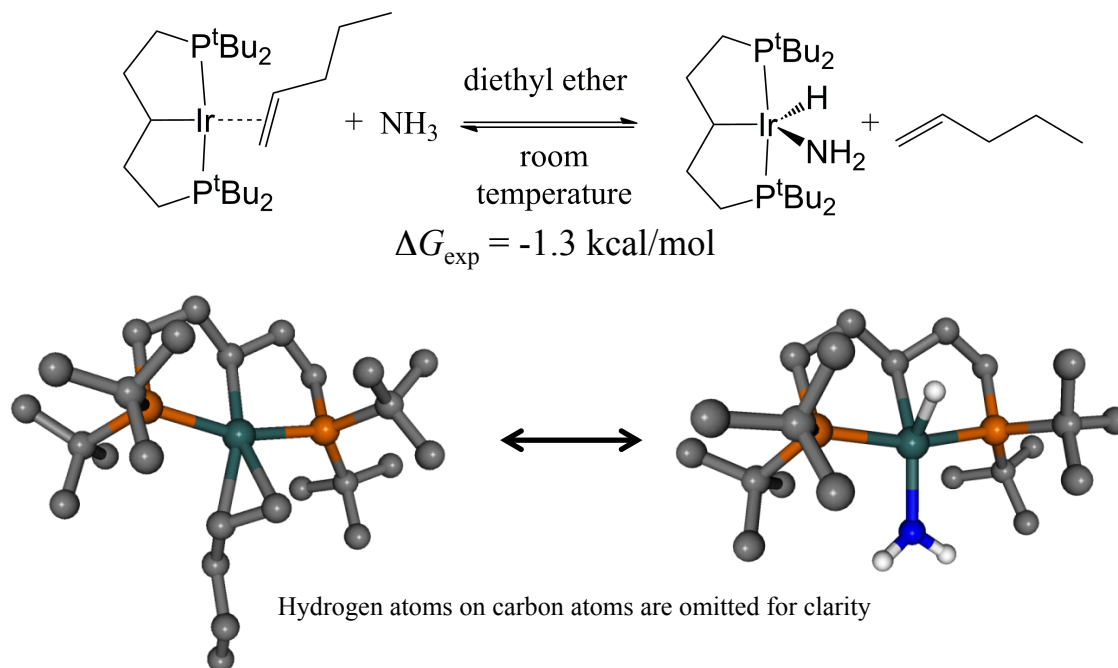
Free energy of reaction and its components (kcal/mol)

	M06-L	M05	M06	PBE	ωB97X	B3LYP
ΔE (gas)	7.0	8.1	10.6	-1.5	-0.1	-6.1
ΔG (gas)	0.4	1.7	4.3	-7.5	-6.9	-11.9
ΔG (liq)	-1.4	0.4	3.0	-8.1	-8.7	-12.9
|error|	**0.1**	**1.7**	**4.3**	**6.8**	**7.4**	**11.6**