Reading Instructions for "Z-Selective, Catalytic Internal Alkyne Semihydrogenation under H_2/CO by a Niobium(III) Imido Complex"[1]

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Sections to Focus on:

- Scheme 5, especially with regard to oxidation states and electron counting
- Scheme 3, along with all of the characterization data on that page (NMR, IR, XRD)
- Figure 2

Questions to Consider:

- Compare and contrast Scheme 1 and Scheme 5. How do the hypothetical mechanisms proposed differ from the traditional mechanisms of catalytic hydrogenation?
- Which path in Scheme 5 do you find preferable, and why? Try and form an argument not based on DFT data.
- Try and justify the observations the authors made in the IR spectra of **2**, **3a**, and **3b**.
- Does the migratory insertion pathway leading to the formyl alkenyl complex (**I-8b**), as observed in the DFT calculations, pose a significant problem to the viability of Path 1?
- In Scheme 3, why does **5** lose its CO ligand in its conversion to **4-d_6**? What about this complex makes it inactive?

Terms to Know:

- Syngas – a mixture of hydrogen and carbon monoxide gases commonly in synthesis
- Isolable – capable of being isolated
- Isotopomer – species which only differ by their isotopic compositions
- BDI - *N*,*N'*-*bis*-(2,6- diisopropylphenyl)-β-Diketiminate

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