

## 5.5: Model Studies for Nitrogen Reduction

Model studies for nitrogen reduction seek to develop coordination compounds that can mimic the activity of nitrogenase, which converts atmospheric dinitrogen into ammonia or ammonium ion. Over the past few decades, there have been more and more reports of dinitrogen complexes, so researchers have clearly figured out some of the factors to accomplish that part of the reaction.

It's one thing to be able to bind a dinitrogen ligand to a metal center, but it's quite another thing to be able to convert that dinitrogen into ammonia. That strong N-N triple bond costs about 200 kcal/mol to break; that's a very high cost to pay and it isn't easy to do. The other part of nitrogen fixation involves formation of the N-H bond; this part of the process could actually be exothermic, and so it might be an easier problem to solve. Most studies aiming to make progress towards ammonia production start with reduction of a metal center so that it in turn will have sufficient reducing power to bind dinitrogen. Acids are then added to supply the protons needed to form N-H bonds. Proposed mechanisms of nitrogen fixation in nature involve a series of electron transfer and proton transfer steps, so the addition of acid seems like a reasonable way to model the process.

### ? Exercise 5.5.1

Assign the oxidation state on nitrogen in the following molecules:

- a) dinitrogen    b) diazene,  $\text{N}_2\text{H}_2$     c) hydrazine,  $\text{N}_2\text{H}_4$     d) ammonia,  $\text{NH}_3$

### ? Exercise 5.5.2

Draw a mechanism with curved arrows and intermediates showing:

- sodium metal reducing Fe(II) to Fe(0)
- binding molecular nitrogen
- protonation to form a diazene complex, containing an  $\text{H}_2\text{N}_2$  ligand.

### ? Exercise 5.5.3

Draw the following possible intermediates of nitrogen reduction:

- a diazene complex
- a hydrazine complex
- a diazenyl anion complex
- a hydrazinyl anion complex
- a bridging hydrazine complex
- a bridging diazene complex (two structures)
- a bridging hydrazinyl anion complex
- a bridging diazenyl anion complex (three structures)
- a bridging hydrazinyl dianion complex (two structures)
- a bridging diazenyl dianion complex

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