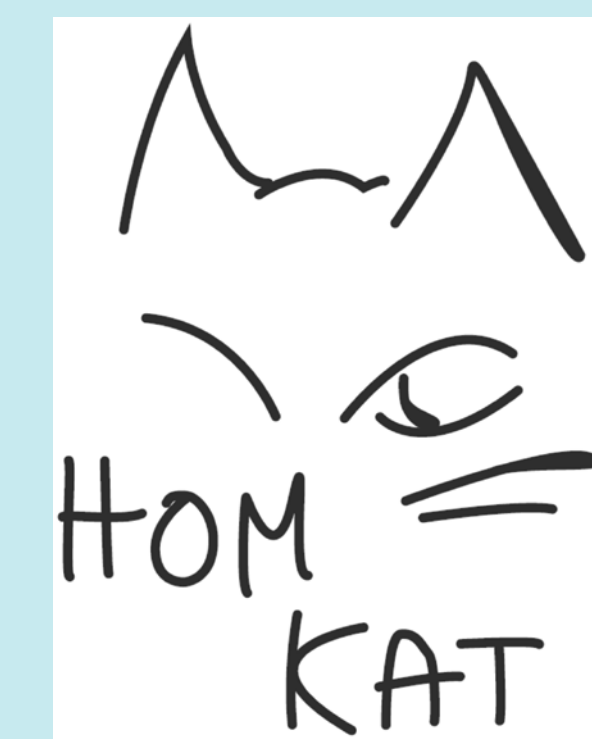


# Cooperative E-H Activation: New Avenues for Catalysis

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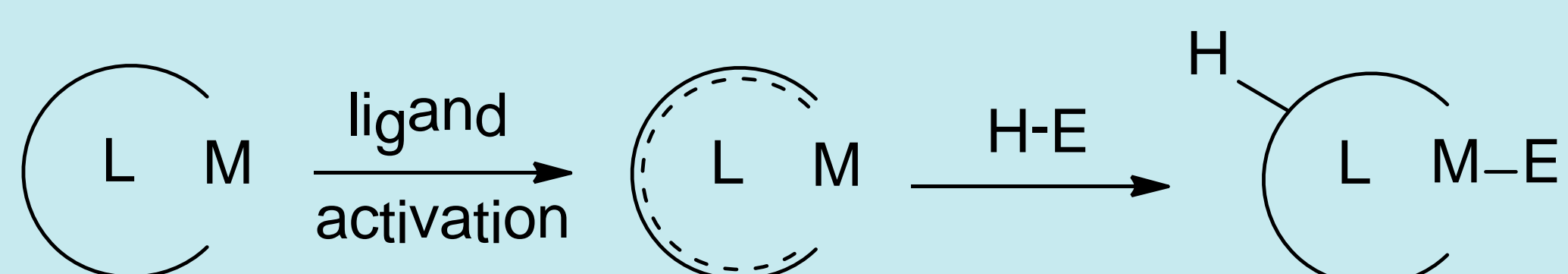
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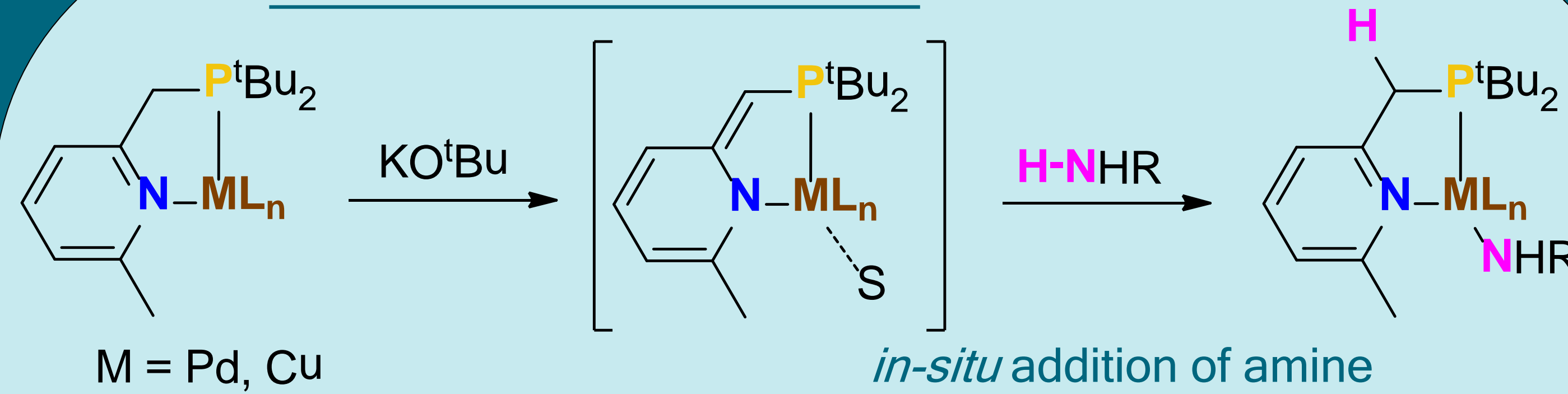
## Introduction

- Cooperative substrate activation is omnipresent in biological systems
- Combinations of 1<sup>st</sup> row TMs and reactive ligands are scarce in synthetic chemistry
- Activation of NH and CH by TMs is of huge interest
  - Development of new catalytic routes for functionalization reactions

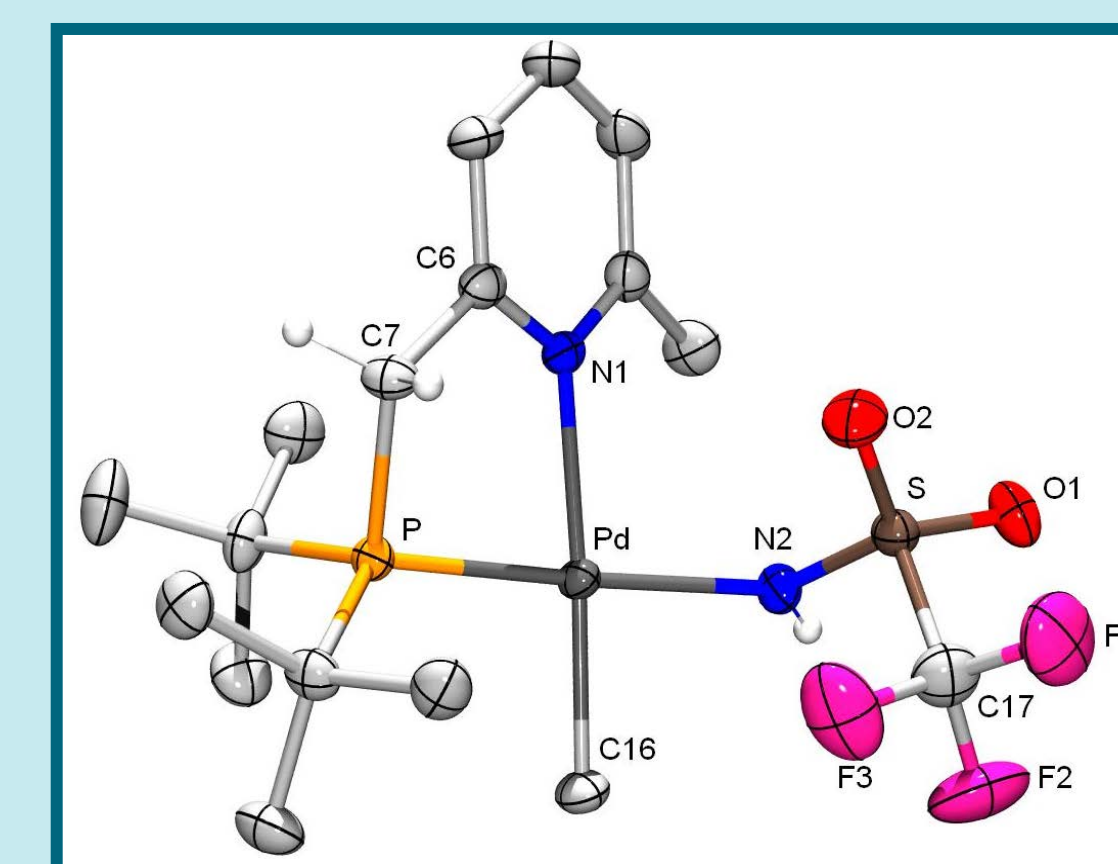
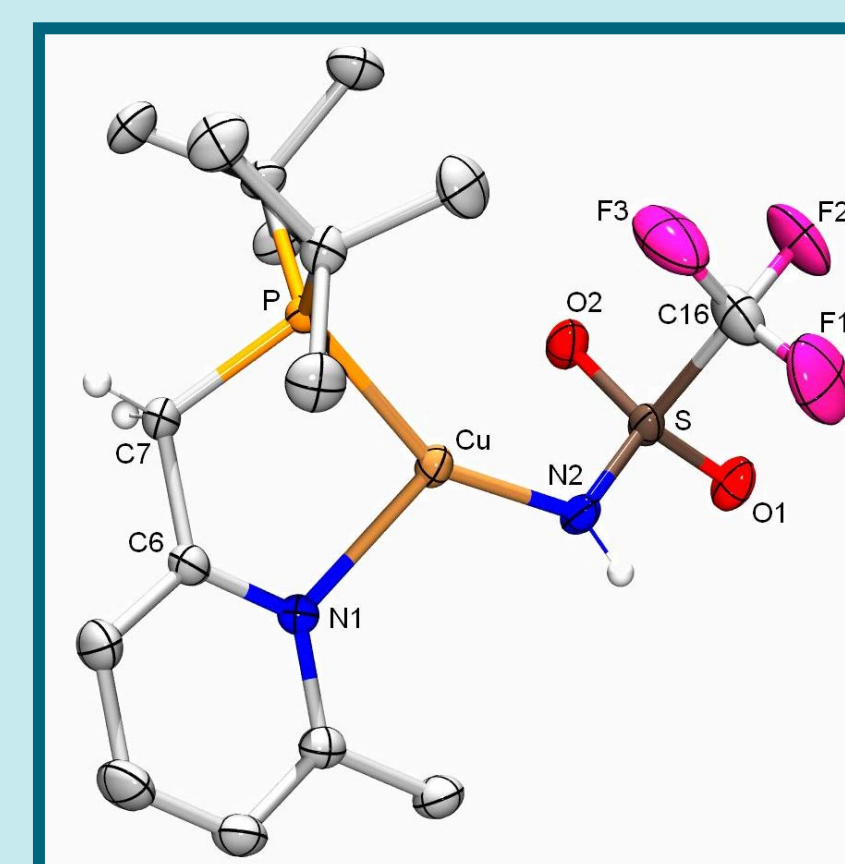
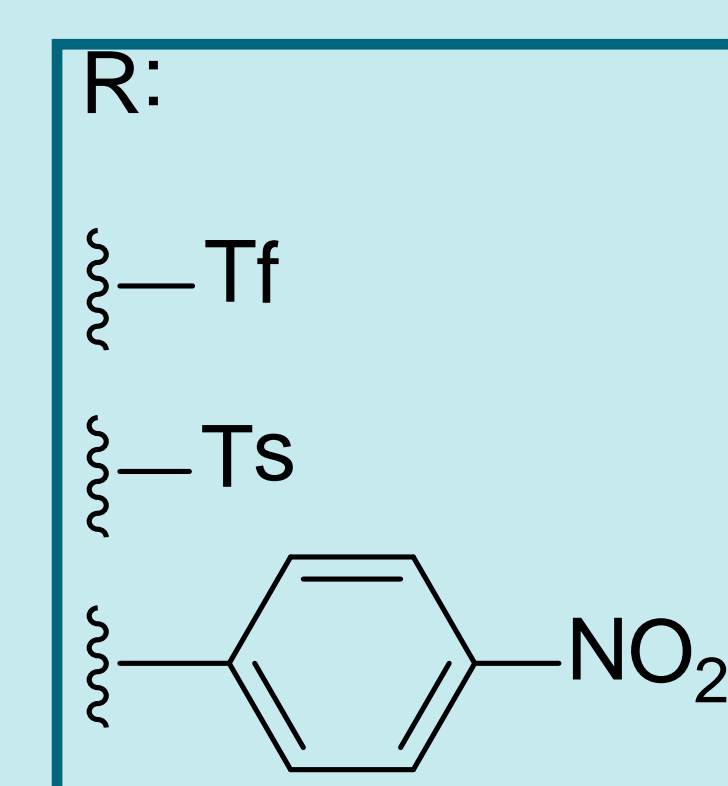
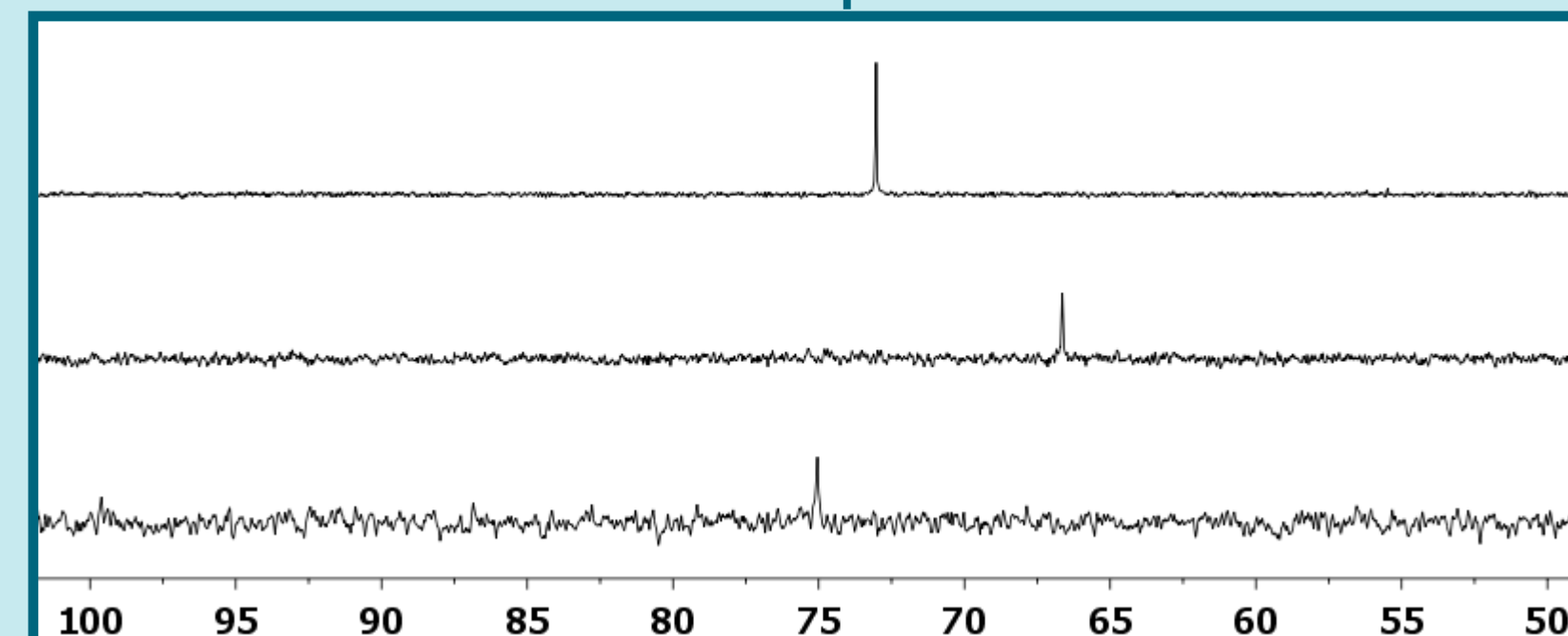


- Goal: Study new cooperative complexes of 1<sup>st</sup> row TMs for activation reactions and additional bond formation

## Activation of Amines

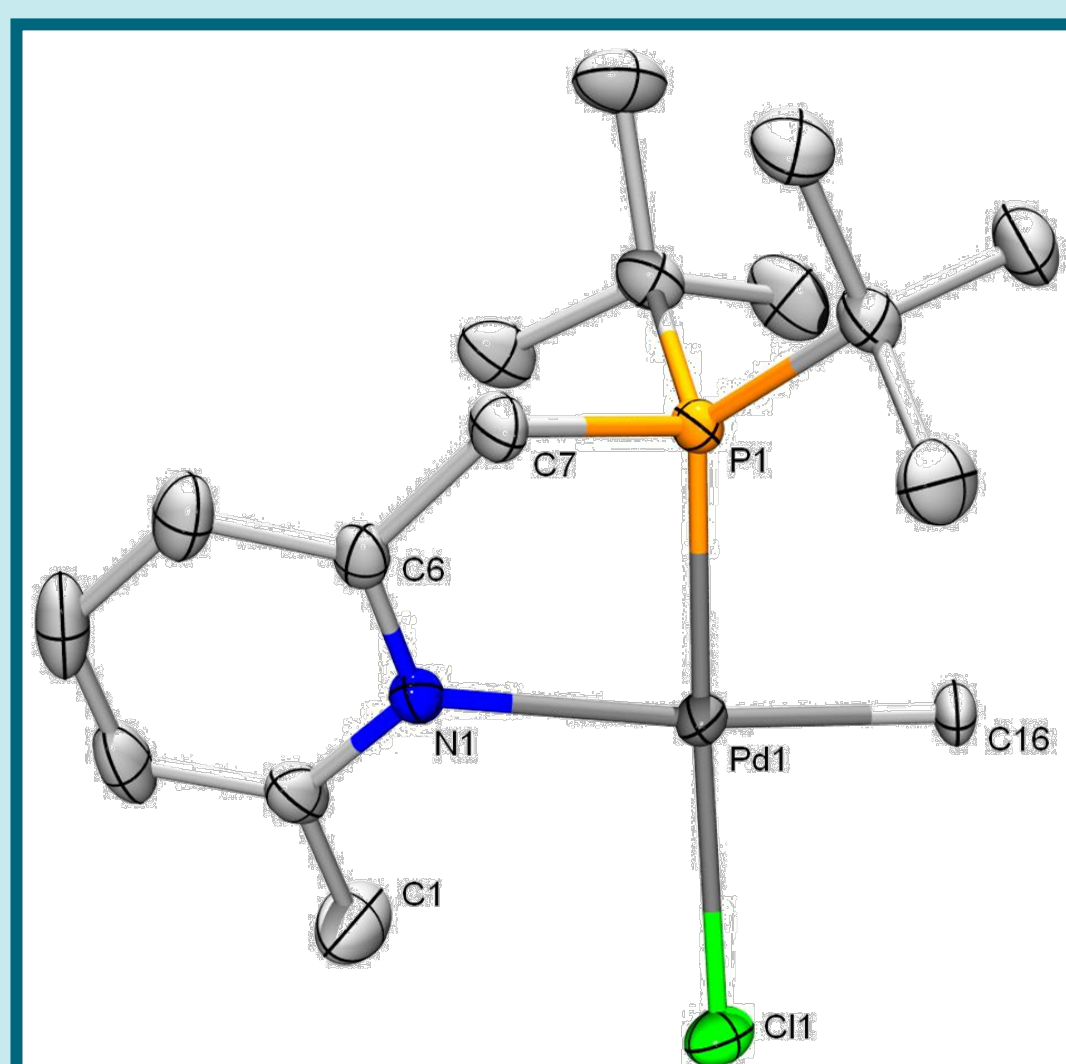
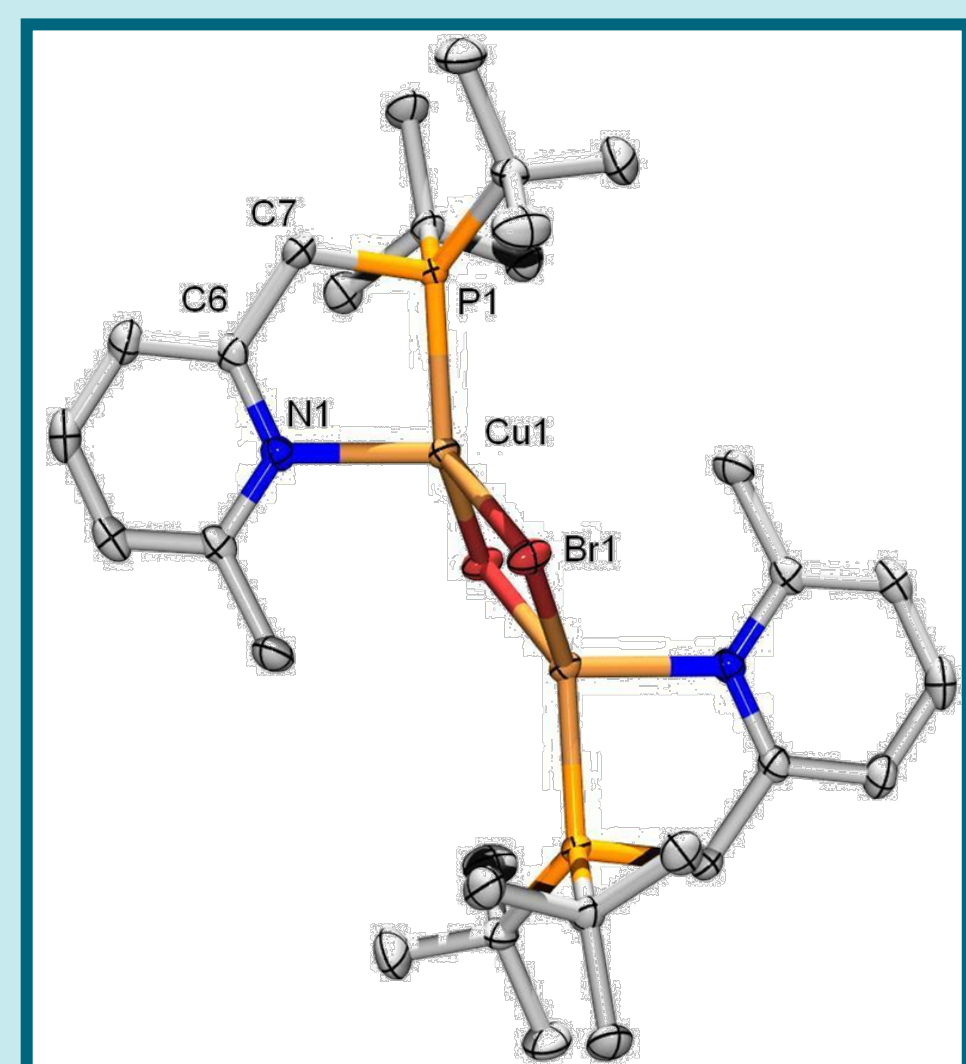
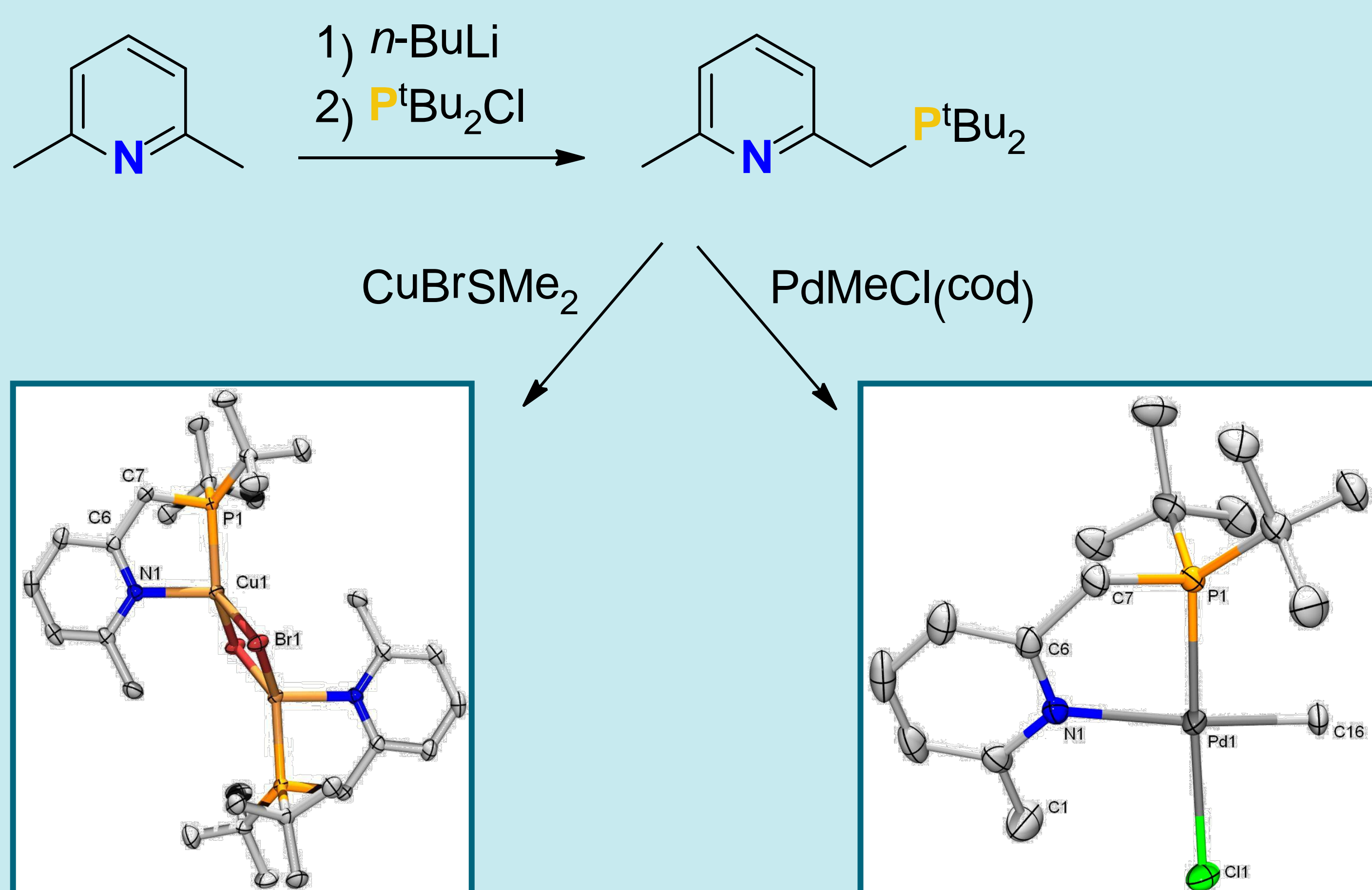


<sup>31</sup>P NMR of 3 Pd-complexes shown above



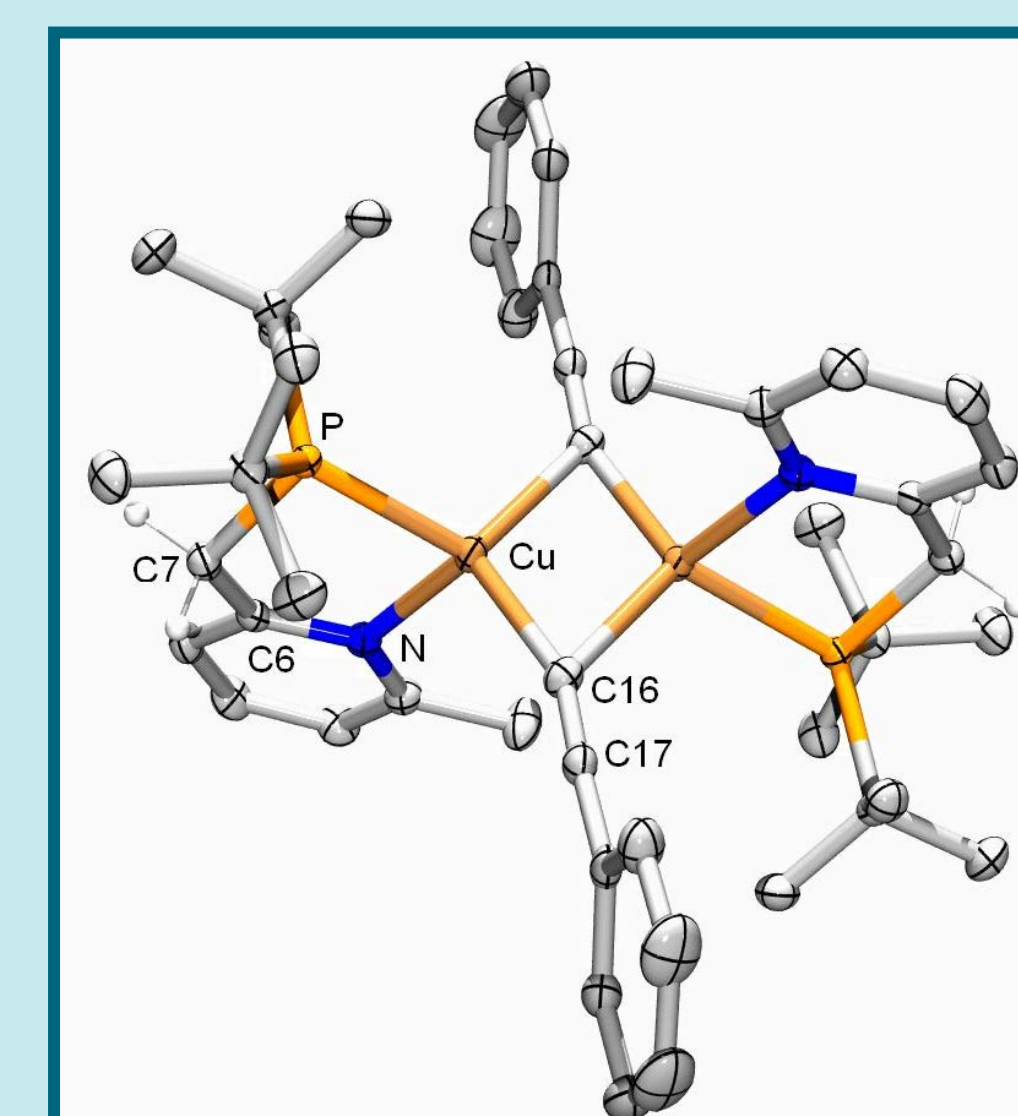
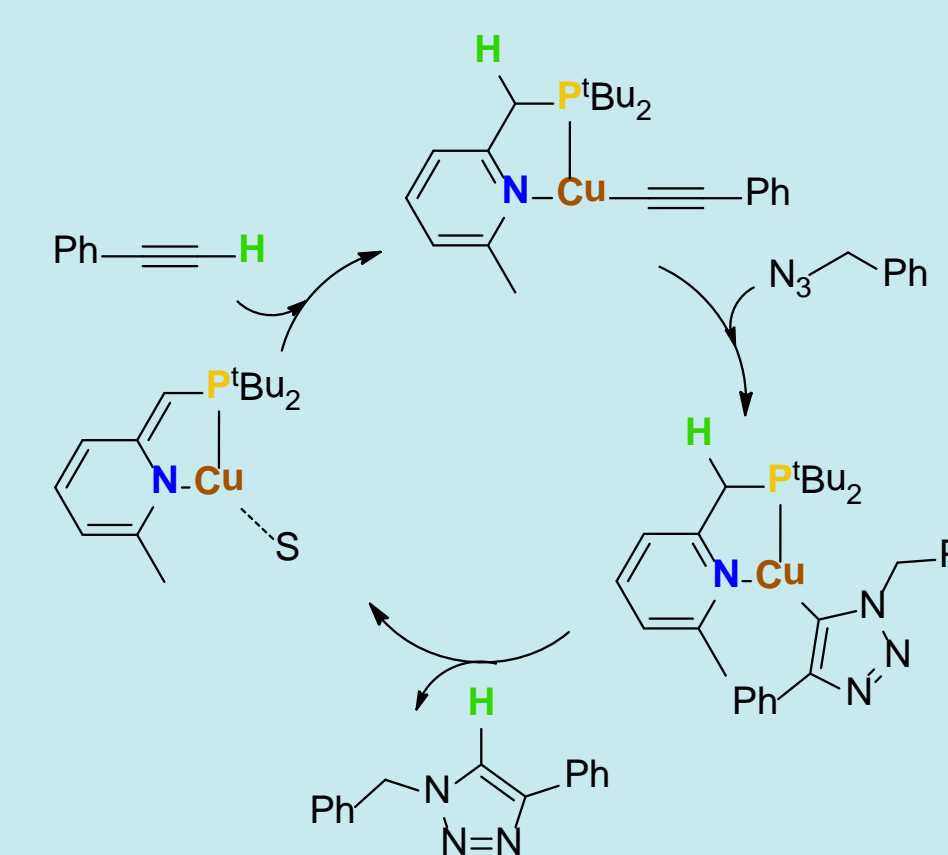
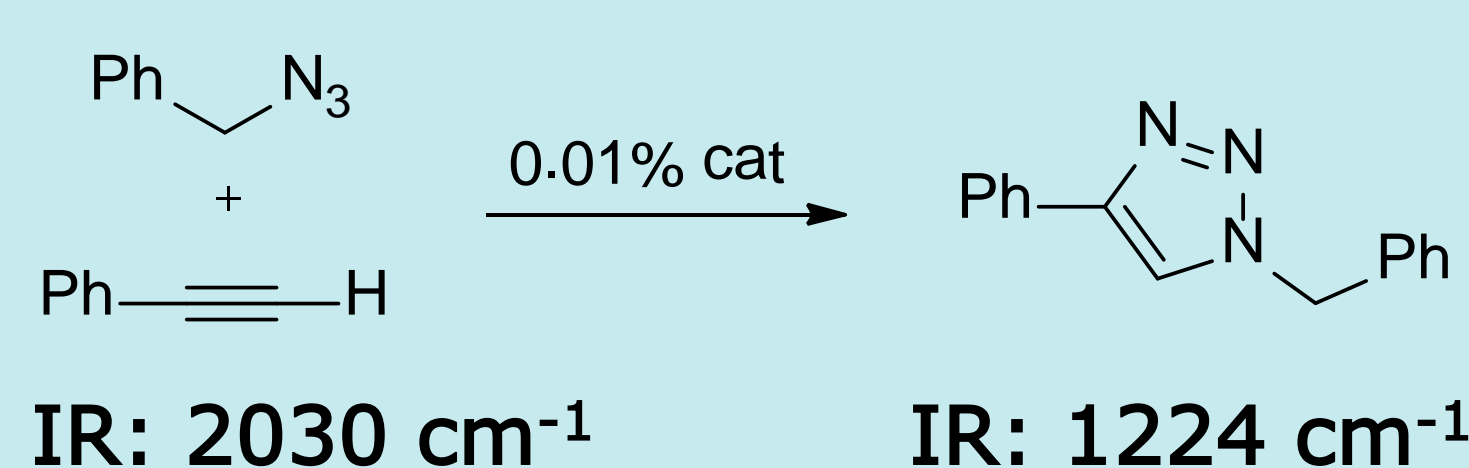
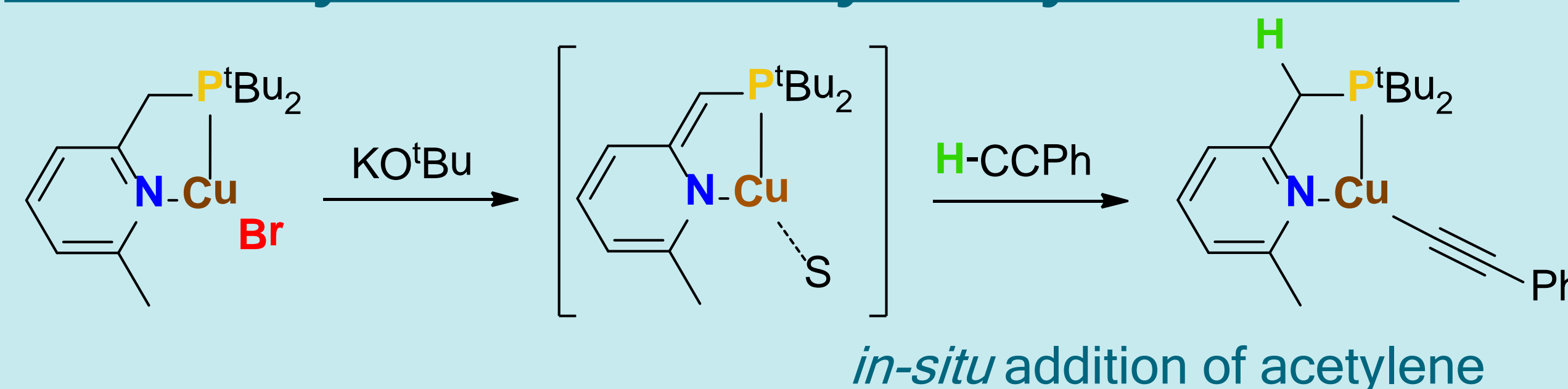
X-rays of activated NH<sub>2</sub>Tf for both Cu (left) and Pd (right).

## Synthesis and Complexation

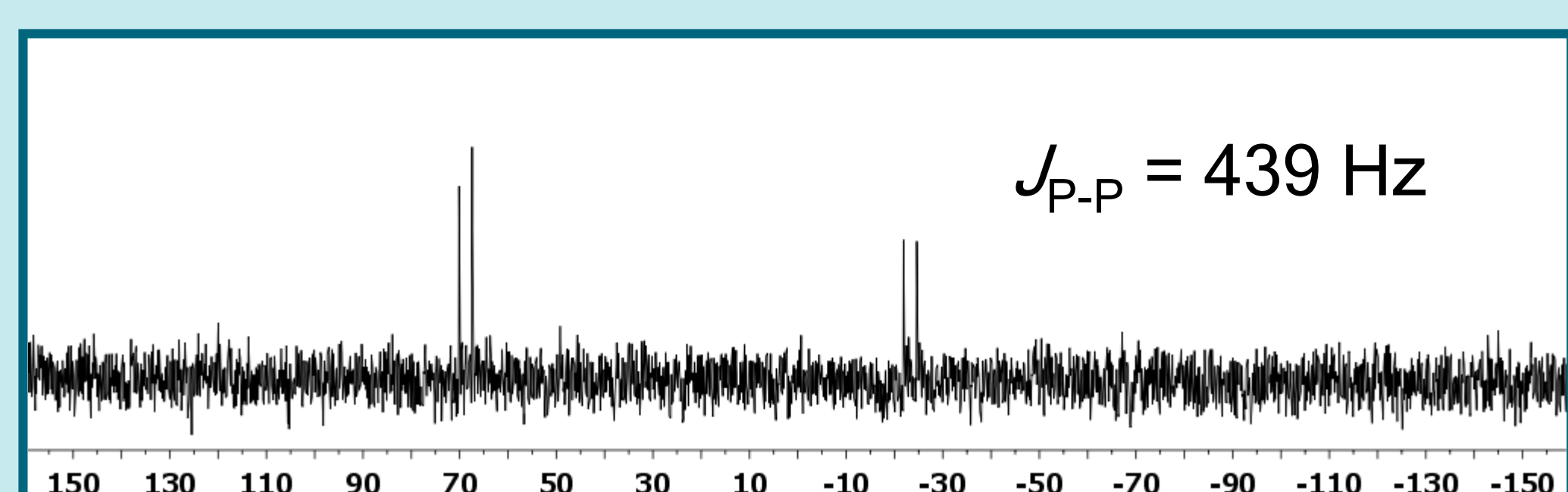
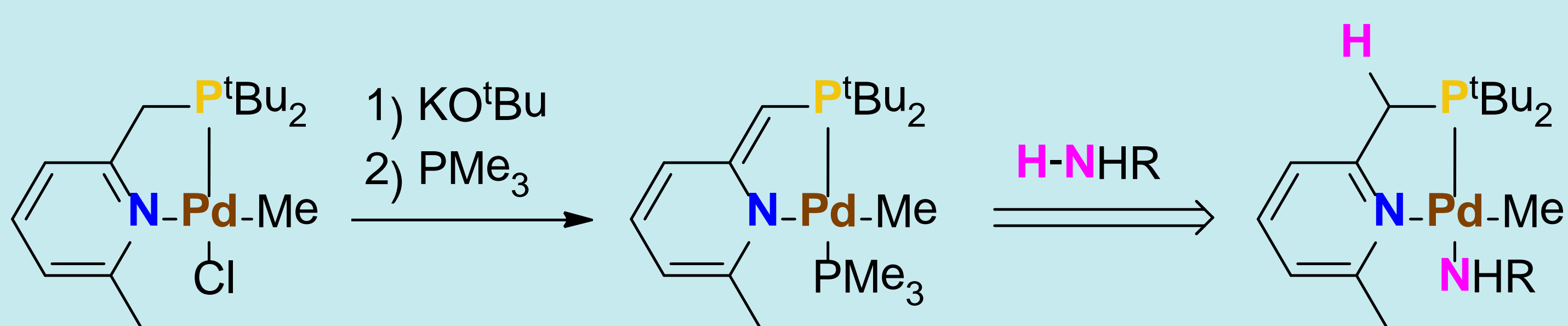


Deprotonated Cu complex is not isolable. Deprotonated Pd complex is isolated, but appears unstable in time. The Pd complex can be stabilized with PMe<sub>3</sub>.

## Cu Catalyzed Azide-Alkyne Cycloaddition



## Stabilization of Deprotonated Complex



## Conclusion & Outlook

- ✓ PN-ligand shows cooperative behavior
  - ✓ Selective N-H activation of acidic amines
  - ✓ C-H activation of phenylacetylene
  - ✓ Application of cooperative ligand in CuAAC reaction
  - ✓ Stabilization of deprotonated complex by neutral co-ligand
  - ✓ Cooperativity of Fe & Ni complexes under investigation
- Explore further reactivity of PN ligand  
➤ Focus on hydroaddition reactions