

## Mechanism of Solid-State C–H Bond Activation by Different Pd(II) Catalysts

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Recent evolution of solid-state synthetic methods has led to their prompt utilization in a metal-catalyzed functionalization of organics.<sup>1,2</sup> An important class of catalytic reactions are palladium-mediated processes for which the C–H bond activation is identified as the first mechanistic step in solution.<sup>3</sup> However, a mechanistic study of the solid-state C–H bond activation is still lacking.

We have studied a mechanism of the ligand-directed C–H bond activation by various Pd(II) catalysts under mechanochemical conditions by *in situ* Raman monitoring and *ex situ* PXRD, NMR and IR methods. Selected Pd(II) precursors, PdCl<sub>2</sub>, PdCl<sub>2</sub>(MeCN)<sub>2</sub>, [Pd(MeCN)<sub>4</sub>][BF<sub>4</sub>]<sub>2</sub> and [Pd(OAc)<sub>2</sub>]<sub>3</sub>, have been employed for solid-state activation of C–H bonds in an azobenzene substrate, Figure 1. Raman monitoring has provided direct probing of the reaction mechanism and revealed how liquid (DMF, MeCN, AcOH and H<sub>2</sub>O) as well as solid additives (NaOAc and NaBF<sub>4</sub>) influence the reactions.

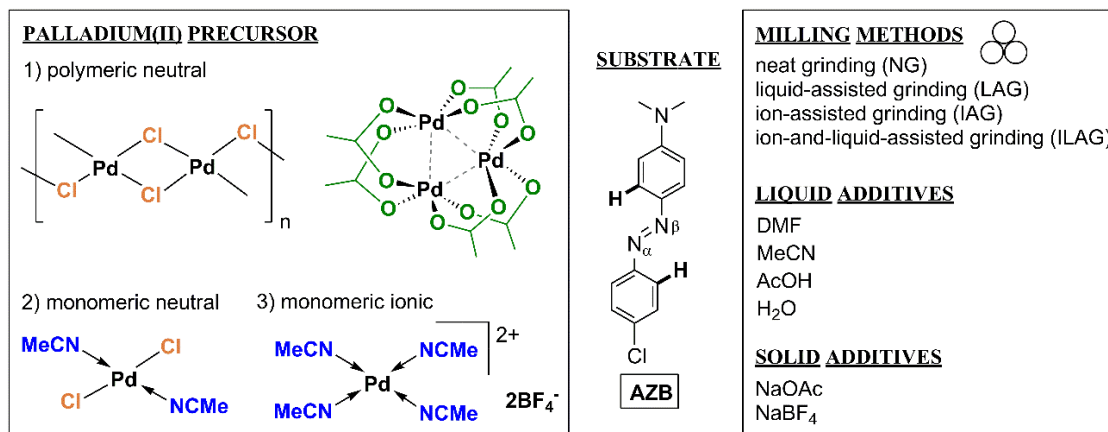


Figure 1. Employed Pd(II) precursors and solid-state methods for the C–H bond activation in **AZB**.

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### References

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