

## Theoretical investigation into NH<sub>3</sub> binding to Dalphos-Pd oxidative addition complexes

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Dalphos ligands, a P,N-based ligand class, have successfully improved the Pd-catalyzed amination. Although the catalyst formation process has been explored, the reactivity and structure of derived intermediates exiting along the catalytic cycle remain unclear. Preliminary PBE-D3(BJ) optimizations combined with DLPNO-CCSD(T) single point energy calculations performed using ORCA program package, revealed that ammonia is able to coordinate to the metal center of the oxidative addition complex (**OAC**), only if a rotation of the square plane around the Pd center is performed. The presente work intends to rationalize what aspects of ligand structure favor NH<sub>3</sub> coordination to the **OAC** and wich ones take the subsequente intermediate to the next steps in the catalytic cycle.