

Supplementary Material

New Bidentate *N*-Sulfonyl-Substituted Aromatic Amines as Chelate Ligand Backbones: Pd Catalyst Generation in C-C Coupling via In Situ and Precatalyst Modes

*Hammed Olawale Oloyede,^{A,B,D} Raymond Akong Akong,^{A,B} Joseph Anthony Orighomisan
Woods,^A Helmar Görls,^B Winfried Plass,^{B,E} and Abiodun Omokehinde Eseola^{B,C,E}*

^AInorganic Chemistry Unit, Department of Chemistry, University of Ibadan, Ibadan, Nigeria.

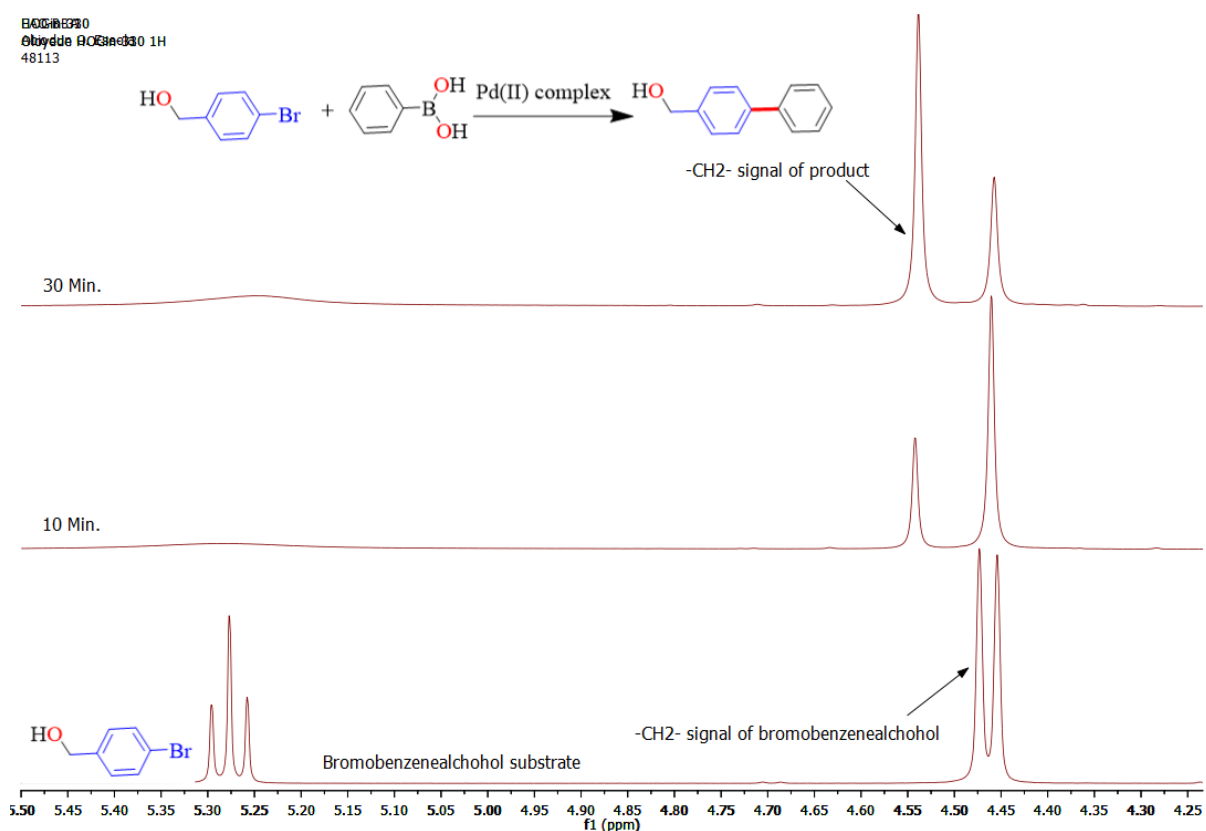
^BInstitut für Anorganische und Analytische Chemie, Friedrich-Schiller-Universität Jena, Humboldtstraße 8, 07743 Jena, Germany

^CMaterials Chemistry Group, Department of Chemical Sciences, Redeemer's University Ede, Osun State, Nigeria.

^DDepartment of Chemistry, School of Science, Adeyemi College of Education, Ondo, Ondo State, Nigeria.

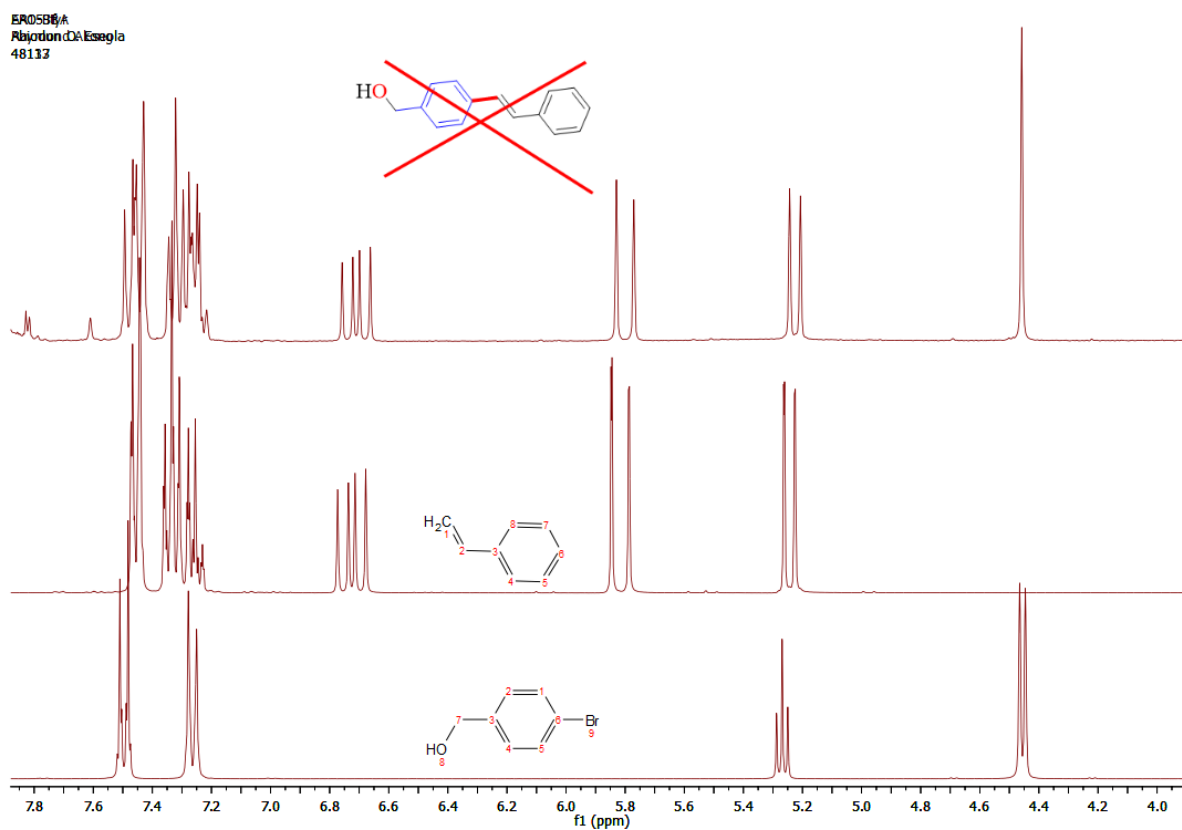
^ECorresponding authors. Email: sekr.plass@uni-jena.de; biodun.eseola@uni-jena.de

Fig. S1: An illustration of the peaks at around 4.4 ppm utilized for estimation of catalytic yield.



It is important to clarify that the 1H triplet signal of the bromobenzenealcohol at about 5.3 ppm (bottom spectra) belongs to the OH function and caused the corresponding splitting of its neighbouring -CH₂- group at about 4.4 ppm. Due to fast proton exchange interactions, this methanoly OH signal as well as the splitting of the -CH₂- is often not observed as is the case for the resultant reaction mixtures after reflux (middle and top spectra). The broad signal of the OH can be seen in the middle and top spectra without splitting.

Fig. S2: Comparison of reaction mixture spectra for Heck coupling in the presence of the ligand free Pd(OAc)₂ with the starting materials (styrene and bromobenzenemethanol).



It is important to clarify that the 1H triplet signal of the bromobenzenemethanol at about 5.3 ppm (bottom spectra of **Fig. S2**) belongs to the OH function and caused the corresponding splitting of its neighbouring –CH₂– group at about 4.4 ppm. Due to fast proton exchange interactions, this methanoly OH signal as well as the splitting of the –CH₂– is often not observed as is the case for the resultant reaction mixture after reflux (topmost spectra).