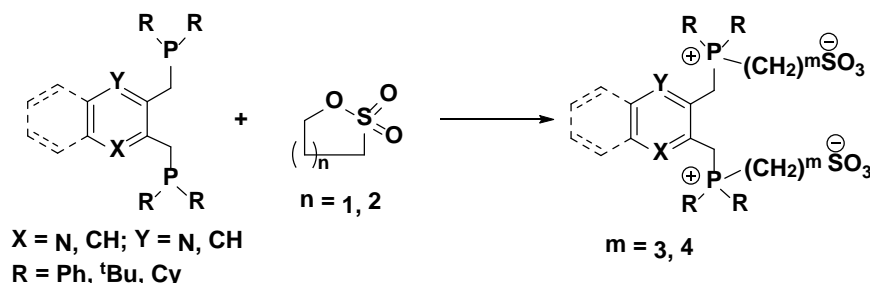


New Zwitterionic Phosphonium Ligands: Application in Telomerization of 1,3-Butadiene

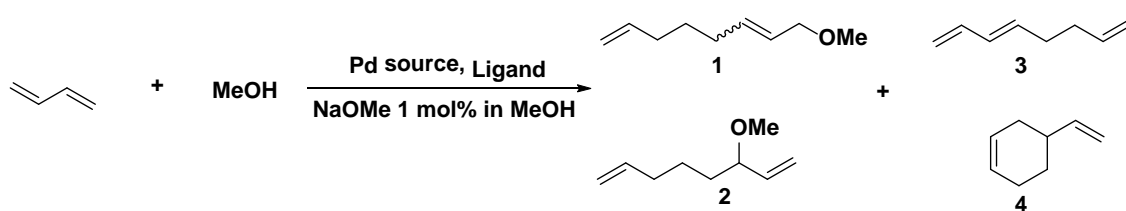
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The design and synthesis of new hydrophilic ligands is an important task for organometallic catalysis. [1] Apart from the steric and electronic control of the metal center, such ligands allow their application in various polar solvents, including aqueous and biphasic systems. Despite of literally thousands of known phosphorus – based ligands, little is known on the application of phosphonium zwitterions in catalysis. Based on our previous work on the synthesis of *N*-heterocyclic backbone based phosphine ligands [2], we were interested in the preparation of novel hydrophilic derivatives of this class of compounds. In this respect, for the first time the synthesis of zwitterionic phosphonium alkylsulfonate ligands and their catalytic applications were described (Scheme 1).



Scheme 1

We demonstrated the chemoselective synthesis of novel phosphonium alkylsulfonates starting from easily accessible *N*-heterocyclic phosphines and commercially available cyclic sulfones in up to 94 % yield [3]. These zwitterionic phosphonium compounds constitute stable hydrophilic pre-ligands. Their catalytic potential is demonstrated in the industrially important telomerization of 1,3-butadiene with methanol (Scheme 2).



Scheme 2

Under optimal conditions in the presence of only 0.001–0.002 mol% palladium loading and corresponding ligand the desired telomers were obtained in up to 87 % yield with chemoselectivities up to 98 %. Obviously these novel pre-ligands have a broad potential for a variety of other catalytic applications. In our presentation we will discuss all results in more detail.

1. K. H. Shaughnessy, *Chem. Rev.* 2009, **109**, 643.
2. A. Pews–Davtyan, X. Fang, R. Jackstell, A. Spannenberg, W. Baumann, R. Franke and M. Beller, *Chem. Asian J.* 2014, **9**, 1168.
3. A. Pews–Davtyan, R. Jackstell, A. Spannenberg, M. Beller, *Chem. Commun.* 2016, **52**, 7568.