Illustration of the Versatility of Organolithium Compounds: the Case of the Direct Arylation of Thiophene

Francesca INGROSSO,[a] Catherine DEMANGEAT,[b] Tarak SAIED,[b] Romain RAMOZZI,[a] Manuel RUIZ-LOPEZ,[a] Armen PANOSSIAN,[c] Frédéric R. LEROUX,[c] Yves FORT,[b] Corinne COMOY [b]

Affiliations: [a] Université de Lorraine, CNRS, LPCT UMR 7019, F-54000 France, [b] Université de Lorraine, CNRS, L2CM UMR7053, F-5400, [c] Université de Strasbourg, Université de Haute-Alsace, CNRS, LIMA, UMR 7042, ECPM, F- 67000 Strasbourg.

Starting from the first synthesis of organometallic lithium compounds in 1917 by Schlenk, a new and extremely rich domain in Chemistry has developed, taking advantage of the strongly polarized C-Li bond that makes these molecules highly reactive, especially as nucleophiles and strong bases. Organolithium compounds play a key role in wide range of applications, ranging from carbolithiation, asymmetric synthesis and deprotonation, to addition reactions.[1,2] Notwithstanding the increasing rationalization of synthetic approaches, the elucidation of the reaction mechanism involving such compounds is still challenging. In this talk, we shall illustrate the interplay between experiments and theory to unravel the reaction mechanism and to optimize the synthetic strategy of the arylation of thiophene using the "aryne coupling" method. An interesting reaction path involving an aryne intermediate, which cannot be isolated through experiments, was described using quantum chemistry calculations. The role played by the ligand and the additives, such as Li salts, was also clarified.

References:
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